BRUKER

topspin

Installation Guide

TopSpin 2.1

Microsoft Windows XP

Version 2.1.0

Bruker BioSpin

Part I

TOPSPIN - Installation and Configuration

Part II

Windows XP - Installation and Configuration

Part III

Tips, Tricks and Troubleshooting

Chapter 1

Introduction

1.1 About this manual

This manual is the TOPSPIN Installation Guide for Microsoft Windows XP and describes the installation of the TopSpin 2.1 under Microsoft Windows XP.

It is available:

- as a hard copy Installation Guide for TOPSPIN 2.1: Windows XP
- as pdf file on the toplevel of the TOPSPIN DVD
- as TOPSPIN Online Help: click ***Help → manuals → Installation Guide***
- as the up to date version on the Bruker web-server:

  `http://www.bruker-biospin.com/documentation_nmr.html`

- Note that this manual does not contain the TOPSPIN Release letter. That is a separate document which is not available as a hard copy but delivered as pdf and text files on the TOPSPIN DVD and also on the Bruker web-server (you can find it at the same URL as the Installation Guide)

  `http://www.bruker-biospin.com/documentation_nmr.html`

This manual is subdivided into an introduction and three main parts. It depends on your local demands which of these are necessary for you at the moment.

The first part shows how to install and configure TOPSPIN and some essential additional software packages. It is recommended to follow the instructions step by step.

Part two describes the scratch installation of Windows XP and some configuration steps for Windows XP, the network and printers. If you want to install Bruker BioSpin TOPSPIN on a PC which is already in use, you can skip this part.

In the last part, you can find some additional information for working with Windows XP and TOPSPIN and also some tips for troubleshooting.

Note that all text-messages and graphics shown in this book are taken from the current version of the respective software products. Small differences to other versions are possible but generally speaking they should be very similar.

If you have any comments or suggestions, or if you find any errors in this manual, please do not hesitate to contact us at:

> nmr-software-support@bruker-biospin.de

1.2 Conventions

Bold-Courier: Windows XP commands to be entered from the keyboard

Bold-Times: Windows XP commands, applications or buttons to be clicked with the mouse

Bold-Courier-Italics: TOPSPIN commands to be entered from the keyboard

Bold-Times-Italic: TOPSPIN commands to be clicked with the mouse

Courier: a file name or directory name

Courier Small Italics: response of the system

Courier Small: the contents of a file

Times italics: any name which is not a file name e.g. hostnames, usernames etc.

< >: place holder

1.3 Safty Regulations

In order to work safety in laboratries with NMR-spectrometers all users have to follow the safety regulations for magnetic, electrical, cryogenic and chemical safety. For detailed information please refer to the safety instructions in the Beginners Guide Manual provided on the TOPSPIN DVD.

1.4 Hardware and software requirements for TOPSPIN

1.4.1 Operating system requirements

TOPSPIN 2.1 on spectrometer computers is supported for:

- Windows XP Professional
- Windows Vista (Business Edition)
- Linux Red Hat Enterprise WS 3 and WS 4

All operating system updates (hot fixes and service packs) at the time TOPSPIN 2.1 was released have been tested and are supported. TOPSPIN 2.1 on Datastations is supported for:

- Windows 2000
- Windows XP Professional
- Linux Red Hat Enterprise WS 3, WS 4 and WS 5

Although not officially supported by Bruker, users reported that TOPSPIN is also running and is used for data processing, respective as storage unit,

- on other Linux systems
  and
- on Windows XP Home Edition.

Bruker BioSpin does not recommend these systems for the use TOPSPIN. Please note, the usage of not supported operating system is at one's own risk!

1.4.2 Special PC Hardware requirements

To run TOPSPIN 2.1 we recommend the following computer hardware:

- PC [1] with CPU Clock $\geq$ 1 GHz

- Memory $\geq$ 512 MB (Windows Vista: $\geq$ 1 GB)
- Video (graphics)-card memory: 64 MB [1]
- Ethernet card (to control a spectrometer, it is essential to have a second ethernet card)
- Mouse with 3-button possibilities
- DVD device [2]

If your hardware does not meet these requirements, TOPSPIN might still run but with a much lower performance.

Furthermore, we recommend setting the display resolution to 1280*1024 or higher.

The Installation was tested on a 'hp workstation xw4400' PC with a 'NVIDIA Quadro FX560' graphics card and two 'Broadcom NetXtreme Gigabit Ethernet' cards.

1.4.3 Spectrometer requirements

TOPSPIN 2.1 is released for datastations, AVANCE (AV), AVANCE-II (AV-II) and AVANCE-III (AV-III) spectrometers.

For upgrade possibilities of your spectrometer with TOPSPIN 2.1, please get in touch with your local Bruker representative.

Hardware components that are TOPSPIN version or operating system dependent are listed below. Components that are not listed here do not need an upgrade for TOPSPIN 2.1.

If your Avance spectrometer does not meet the above specifications, please get in touch with your local Bruker representative for your upgrade options.

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1. TOPSPIN 2.1 only runs on x86 based PC's. It does not support 64bit architecture.
1. It is recommend not to use shared memory graphics, because in some cases memory problems could be observed.
2. TOPSPIN 2.1 is delivered on DVD's with "-r" format.

1.4.3.1 AVANCE and AVANCE-II spectrometers (AQS based)

- **CCU**

LINUX, independent of the TOPSPIN Version	
CCU	**required minimum EC level**
CCU 10 (part # H9503) EC level 00 to 19	**06**
CCU 10 (part # H9503) EC level > 19	**22**
CCU 11 [1] (part # H9503V1)	**00** (recommended **01**)

1. Note that CCU 11 also exists for AQX/AQR spectrometers.

Windows, independent of the TOPSPIN Version	
CCU	**required minimum EC level**
CCU 10 (part # H9503)	requires no specific EC level
CCU 11 [1] (part # H9503V1)	**00** (recommended **01**)

1. Note that CCU 11 also exists for AQX/AQR spectrometers.

- **FCU 3**

FCU 3	**required minimum EC level**
part # H5822 (64k memory)	**04** (recommended **07**)
part # H9598 (256k memory)	**02** (recommended **05**)

- **FCU 4**

FCU 4	required minimum EC level
part # H9727	requires no specific EC level
part # H9773	requires no specific EC level

- **RCU**

RCU [1]	required minimum EC level
RCU 1/2 (part # Z003678)	requires no specific EC level
RCU 1/3 (part # Z022488)	requires no specific EC level

1. AVANCE (AV) spectrometers ony

Multiple Receiver RCU [1]	required minimum EC level
RCU 1/2 (part # Z052488)	requires no specific EC level
RCU 2/4 (part # Z062488)	requires no specific EC level
RCU 3/4 (part # Z072488)	requires no specific EC level
RCU 4/4 (part # Z082488)	requires no specific EC level
RCU 1/5 (part # Z003206)	requires no specific EC level
RCU 2/5 (part # Z003207)	requires no specific EC level
RCU 3/5 (part # Z003208)	requires no specific EC level
RCU 4/5 (part # Z003209)	requires no specific EC level

1. AVANCE (AV) spectrometers ony

- **TCU 3**

TCU 3	required minimum EC level
part # H5813 with EC level between 00 to 19	**09** (recommended **12**)
part # H5813 with EC level $\geq$ 20	**28** (recommended **31**)
part # H5813V1	**any** (recommended **01**)
part # H5813F2	**any** (recommended **01**)
part # H5813F3	**any** (recommended **01**)

- **RX22**

RX22	required minimum EC level
part # Z002810	**any** (recommended **08**)
part # Z012810	**any** (recommended **02**)
part # Z032810	**any** (recommended **01**)

1.4.3.2 AVANCE III spectrometers

- **IPSO 19"**

IPSO 19" H9987	required minimum EC level
Baseboard part # H12519	**03**
TX-board (F-/T-/G-Ctrl) part # H12538F1	**01**
TX-board (F-/T-/G-Ctrl) part # H12538F2	requires no specific EC level
RX-board (R-Ctrl) part # H12532	requires no specific EC level
PCI-board part # H12524	**01**

- **IPSO-AQS**

IPSO-AQS H9984	required minimum EC level
IPSO-ACQ host part # H12547	requires no specific EC level
IPSO-ACQ acq part # H12549	requires no specific EC level
PCI adapter board part # H12557	requires no specific EC level
HR-board part # H12553	requires no specific EC level
FTMS-board part # H12555	requires no specific EC level

- **DPP1**

DPP1	required minimum EC level
part # H12513F1	requires no specific EC level

1.4.4 Software requirements

!
- Microsoft Windows Vista, Windows XP (SP2) or Windows 2000 (SP4) [1] for TOPSPIN $\geq$ 2.1 [2]

- on DVD: 'TOPSPIN 2.1'
    - TOPSPIN
    - Flexlm License Manager [see Chapter 7]

- For spectrometer control the following version must be used:
    - Hummingbird NFS Server Version 7.1 [3] (*CD*: TOPSPIN NT Toolkit) [see Chapter 4]

- For NMR-GUIDE:

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1. Windows 2000 only for Datastations (for further information see chapter 1.4.1).
2. TOPSPIN requires a NTFS filesystem on the partition where the Topspin is installed and a NTFS filesystem on all partitions where TOPSPIN data are stored [see chapter 14.1].
3. The NFS Server is only required for AVANCE and AVANCE-II spectrometers.

- • Internet Explorer ≥ 6.x (*CD:* Microsoft Windows XP)
- • For TOPSPIN Online Help and NMR GUIDE
  - • A PDF viewer (e.g. Adobe Acrobat Reader [see Chapter 5])

1.5 Important Windows configurations

This Installation Guide for TOPSPIN refers to the following configurations for Windows XP. Several functions (e. g. Control Panel, Start menu, Windows Explorer) can be configured in a *Classic view*-mode or *Category view*-mode (Windows XP style). These modes are not only different in style. They can be different in the way commands are entered.

1.5.1 Configure the Start Menu

For this manual the Start Menu is configured in the Windows XP style.

- • Click the RIGHT mouse button on the Taskbar → click **Properties**
- • Click **Start Menu** → click **Start Menu** → click **OK**

1.5.2 Configure the Control Panel and the Windows Explorer

For this manual the Control Panel and the Windows Explorer are configured in the *Classic View* style.

- Click on the left side on *Switch to Classic View*
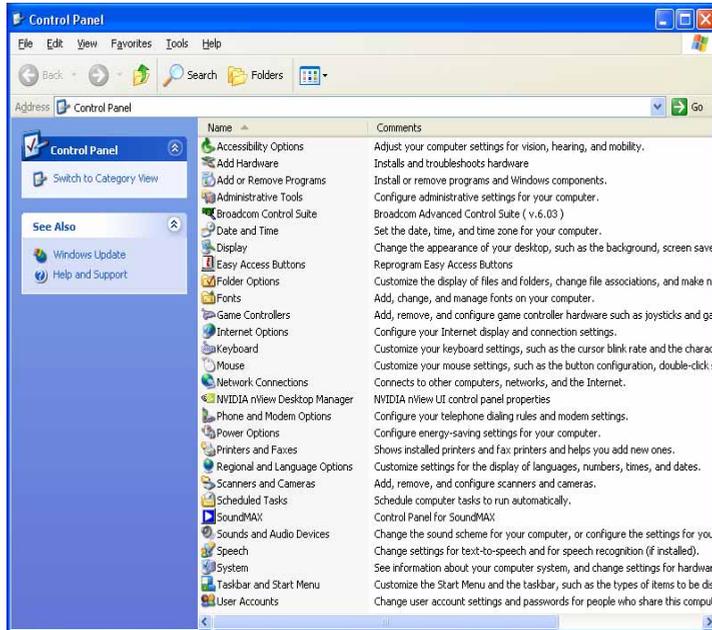
Chapter 2

Express Installation and Configuration of TOPSPIN

2.1 About this chapter

This chapter gives a brief description of how to install Bruker BioSpin's TOPSPIN.

This chapter is directed to users who would like to install TOPSPIN 2.1 on a PC, on which XWIN-NMR or a version of TOPSPIN is already installed and configured correctly. Therefore this chapter provides an overview and provides not information on all aspects of configuring Windows XP and TOPSPIN.

For more details on the installation see chapter 6.4.

For more details on the TOPSPIN commands like *cf*, *expinstall*, etc. please refer to the description of this command in the Acquisition Reference manual.

2.2 Installing TOPSPIN

The main decision you have to make during installation is where do you want to install the new TOPSPIN version. If you a have previous NMR SUITE or TOPSPIN installation on this PC available, you can either:

- install the new version in parallel to the previous one
  (e.g. old in `C:\Bruker\TopSpin1.3` and new in `C:\Bruker\TopSpin2.1`)

  or

- install the new version in the same directory as the previous one
  (e.g. old in `C:\Bruker\TopSpin` and new in `C:\Bruker\TopSpin`)

The installation in parallel has the advantage, that the previous version remains unchanged. After a parallel installation you can start working with the new version and if you want to go back to the previous version for whatever reasons you can just start and reuse it.

The installation of TOPSPIN 2.1 offers an automatic import of your individual configuration of a previous version, so that there is no advantage to install the new version in the same directory as the old one.

1. Log in as a Local Administrator
2. Close ALL WINDOWS on the desktop
3. Insert the DVD 'TOPSPIN *2.1*'.
4. Start of the installation
   - If the automatic start of the DVD is enabled, the window described in the next step appears automatically, go to step 5
   - If this window of the next step does not appear automatically, autorun is probably switched off (see chapter 10.3) or open the Windows Explorer, go to the DVD device and double-click `install.cmd` [1].
5. The windows *Welcome to the TOPSPIN Setup* will appear: → Click **Next**
6. A window *Release Letter TOPSPIN* will appear:
   a) Please read the NMR Release letter! You can find there all information about news and bug fixes of the current version.
   b) Close the Release Letter by clicking the **X** button in the upper right corner
   - Select the destination directory for TOPSPIN.
     a) Accept the default destination
     b) or browse to another destination.

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1. Please note that there is also a file called 'install' on the DVD. This file is the installation script for Linux, under Windows you have to click on the file 'install.cmd'

- Enter an installation path which does not exists so far, e. g. **C:\Bruker\topspin2.1**
- or browse to another existing installation path.
- Click **OK**
- Click **Next**

7. A window *Select the setup type* will appear:

a) Select the setup type. Do one of the following:

- Select *Data Processing, Acquisition and Automation* if you want to use TOPSPIN for spectrometer control. This will install **Diskless** automatically.

- Select *Data Processing* if you want to use TOPSPIN for data processing.

- *Customized setup* (allows components selection) if you want to install selected programs only.

    A window 'Product selection' will appear. Select the packages which you want to install (note that DISKLESS is only required if your PC controls a spectrometer or you want to configure it like this.

b) Click **Next**

8. A window '*Question*' will appear if Windows XP Service Pack 2 is installed and enabled on your system. If you click **Yes** on the installation configure the firewall [1] for you [2].

9. A window '*Select Components*' will appear. You can either import no spectrometer configuration, or browse for a spectrometer configuration or select one of the configurations you get offered within this window [3].

- Click **Next**

10. A window '*Set NMR Super User*' will appear:

a) Do one of the following:

- Accept the default NMR Superuser (Administrator) or

- Enter a special user for this purpose, e.g. named *nmrsu* or

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1. The firewall must be configured to enable spectrometer access.
2. If you click on **No** an Administrator can do it any time later, running *<topspin-home>\prog\bin\Utilities\Miscellaneous\setfirewal.cmd (see chapter 8.9).*
3. The installation process will offer all configurations which are available in the TOPSPIN / XWIN-NMR installation that are defined in the registry.

- • Enter any other user

Under Windows the username must be the name of an existing user. For further details check chapter 6.2.

   b) Click **Next**

11. A window '*Password Input*' will appear [1] (for more details about this feature see chapter 6.2):

   a) Do one of the following:

- • Type in the NMR ADMINISTRATION PASSWORD
- • Re-enter the NMR ADMINISTRATION PASSWORD

   b) Click **Next**

   → The installation of TOPSPIN will start now.

12. A window '*Setup is complete*' will appear:

- • You will be asked if you want to restart the computer:

   a) Click **Yes I want to restart my computer now**

   b) Click **Finish** (to reboot the computer)

13. After the PC has booted up, press the reset button on the CCU or turn it on with the key if it was switched off. Don't forget to execute **cf** and **expinstall** (if necessary; see chapter 2.3).

The following information is for the *Customized setup:*

- • It is strongly recommended to accept the default path for the flexLM installation: 'C:\flexlm' ! If you choose a user defined path, it may cause some problems with other applications using the FlexLM.

2.3 Configuring TOPSPIN

The idea of this chapter is to give you some guidelines to configure TOPSPIN for using it on a workstation for data processing, or for operating a spectrometer. We do not discuss the commands in detail here. For a full description refer to the TOP-

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1. Certain commands like **cf** and **expinstall** ask for the NMR ADMINISTRATION PASS-WORD.

SPIN manuals.

Start TOPSPIN:

- Click the icon TOPSPIN on the desktop, or
- Click **Start → All Programs → Bruker TOPSPIN → TOPSPIN<vers.>**

After the first startup of TOPSPIN a window 'LICENSE' will appear:

a) Please read the license agreement for Bruker TOPSPIN !

b) If you agree, please click **I Accept**.

After the first startup of TOPSPIN a window 'Configuration check' will appear.

You have the possibility to configure the software (depending upon the hardware of your spectrometer). If you do this, you are probably in one of five situations:

1. You want to configure a processing-only-PC with a default configuration on a datastation → go to chapter 2.3.1 (see also chapter 8.1.3)

2. You have just installed the software in a new directory and the old spectrometer configuration of the software is still known to the new version → go to chapter 8.1.1

3. You want to configure a processing-only-PC like your spectrometer-PC, so you have the spectrometer configuration on another computer → go to chapter 8.1.2

4. You have to configure the software on a new hard disk without a backup of the spectrometer configuration, so you have no configuration files → go to chapter 8.1.4

5. You have a new spectrometer hardware component, so you have no configuration file → go to chapter 8.1.5

If you would like to take over the configuration of an existing XWIN-NMR or TOPSPIN installation into TOPSPIN 2.1, please check chapter 8.2.

2.3.1 If you want to use a default configuration on a datastation

A default configuration can be used on a PC that is used for processing only. It is automatically performed (no `cf` required) during the installation of TOPSPIN on a new computer, a new disk or in a new TOPSPIN installation directory. The default configuration names are *Bruker_default_av500* (corresponds to an Avance 500 MHz spectrometer) and *Bruker_default_avanceII300* (corresponds to an Avance II 300 MHz spectrometer).

For data processing, the automatic default configuration is sufficient. If, however, you want to use AU programs, you must execute **`expinstall`** and select *Installation for Datastation (Default)*.

For further details please refer to the respective chapters (see chapter 8.1.2).

2.3.2 If your PC controls a spectrometer:

1. Be sure that the spectrometer is booted (see chapter 6.4 and also 15.5.3)

2. Open a dataset
   - Type **`new`** and create a new dataset.
   - You can also select a dataset (e.g. `exam1d_1h`) acquired with another TOP-SPIN or XWIN-NMR version

3. Enter **`cf`** (The command **`cf`** now configures the software according to the hardware of your spectrometer.)

   a) A window will appear:
      `Password request. Please enter the NMR administration password`

      Type in the NMR ADMINISTRATION PASSWORD. Click **OK**.

   b) A window will appear:
      `Spectrometer configuration: ...`

      Most likely you will select an existing configuration and press **Edit** to confirm this configuration.

   c) A window will appear:
      `Edit configuration. ...`

      The selected configuration is displayed. Choose whether to configure it as a spectrometer or datastation. Choose the type of your spectrometer e.g. **`AVANCE`** → **ENTER**. Check or type in the 1H frequency of the magnet e. g. **`500.13`** → **ENTER**. Use the debug mode only in case of troubleshooting.

   d) If a `mod hconfserver` information window appears:
      - your spectrometer has not a BSMS rack with ECLB board: you may ignore this warning. Nevertheless please check the Configuration summary (`uxnmr.info` file) if all units are listed.
      - your spectrometer has a BSMS rack with ECLB board: please check if the DHCP server is running. If you cannot start the Bruker DHCP ser-

vice please see chapter 15.6.

e) A window will appear:
   Specify the channel to which external devices are con-
   nected. The RS232/485 channel for external devices-
   Table appears.

   Check if the tty-numbers of the hardware components are set correctly.

f) A window '*Additional configuration*' will appear:
   Security check. Enable peak power check (POWCHK).

   • Choose the options if you want to use this security options. *Powchk*
     and *Pulchk* require special probes and *cortab*. If in doubt contact your
     local Bruker representative, please.

   Sample changer configuration. Should the Sample Chang-
   er control the Lift? (yes/no)

   • The answer depends on how the air flow is connected, normally you
     will answer: **yes** → **ENTER**

   Delay between SX and next command [sec]?

   • Type in the length of the delay e. g. **10** → **ENTER**

g) The *nuclei-table* appear

   Check if the frequency of the nuclei are set correctly. If in doubt click **Re-**
   store then click **Save**

h) A window 'Edit spectrometer configuration' will appear:
   Check if the preamplifier connections are set correctly and click **Save**..

i) The results of **cf** appears in a text window. Check this list carefully and
   compare the result with an list from an earlier configuration (if available)
   click **Print** and store the paper output with your other spectrometer
   documentation, then click **OK.** *These data are saved in*
   <TOPSPINHOME>/conf/instr/<spect>/uxnmr.info.

! **If during 'cf' an error message occurs that invites you to do a firmware**
update check chapter 8.6

After finishing **cf** the window '*config*' will appear showing a list of configura-
tion steps. You will be asked for the NMR ADMINISTRATION PASSWORD
several times:

• Continue with **expinstall**

   a) Type in the NMR ADMINISTRATION PASSWORD and **ENTER**

b) Click **Next** if you either have not modified Bruker BioSpin Parameter files, AU-programs and Pulse-programs or if you have archived them in a different directory. Your individual Parameter files, AU-programs and Pulse-programs etc. that are named different to the original Bruker BioSpin files will not be destroyed during the installation.

c) A window appears: Check *Installation for Spectrometer* → Click ***Next***

d) In the appearing window: Check *the required system* → Click ***Next***

e) In the appearing dialog box: Select the spectrometer configuration name → Click ***Next***

f) In the appearing dialog box: Check the items you want to install or, accept the default selection → Click ***Next***

g) In the appearing dialog box: Select the default printer and plotter and the desired paper format → Click ***Next***

h) In the appearing window: Enter the desired spectrometer frequency, acquisition mode and pre-scan-delay or, accept the default values → Click ***Next***

i) In the appearing information box: Check the configuration selection and, if it is correct → Click ***Finish***
While Expinstall will be executed, you can configure the next configuration programs.

- Continue with `edsolv`

    Check the list of lock solvents → click **Save** if it is correct → Click **Close**

- Continue with `edhead`

    Select the current probe → click ***Define as current probe*** → Click ***Exit***

    A window 'Edit Spectrometer Parameter' will appear:
    Check if the connections between preamplifier and probe are set correctly → click **Save** if it is correct → Click **Close**

- Continue with `edprosol`

    Check the parameters for your observed nuclei, and if necessary change and/or recalculate them → Click *Save* to store to disk → Click ***Exit***

- Continue with `edlock`

    Check the lock table values (field, lock phase, ...), change them and click *Save* if necessary, otherwise click ***Abort***

- Continue with `edscon`

Check the spectrometer constants, change them and click *Save* if necessary, otherwise click *Cancel*

- After finishing the configuration a window `cron check` appears. Click on **`Automatic backup`** to set up an periodically backup.

After **`cf`**, **`expinstall`**,... have finished insert a sample and make sure that you can lock on the lock solvent. Type **`ii`** and read with **`rpar`** a standard Bruker BioSpin parameter file (e. g. 'rpar PROTON all'), type **`getprosol`**, **`rga`** and **`wobb`** and collect a normal ^{1}H NMR spectrum.

2.3.3 If you want to configure a processing-PC like your spectrometer-PC:

If the PC does not control a spectrometer but is used in connection with a particular spectrometer, e.g. for setting up experiments, processing and or plotting, you should configure it as that spectrometer (see chapter 8.1.2).

Part I

TOPSPIN - Installation and Configuration

Chapter 3

General Installing Information

3.1 Installation order

A complete new installation on a PC connected to a spectrometer involves the following steps:

1. Installing Windows XP (see chapter 11.1)
2. Installing Windows XP Service Pack (see chapter 11.2)
3. Installing the Graphics driver (see chapter 11.3)
4. Configuring the network (see chapter 13)
5. Installing a printer (see chapter 14)
6. Installing a PDF viewer (see chapter 5)
7. Installing NFS Server (see chapter 4.3) [1, 2]
8. Installing TOPSPIN (see chapter 6.4)
9. Configuring NFS Server (see chapter 6.6) [2]

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1. Note for Windows XP SP2 users with enabled firewall: If you have installed the NFS server after TOPSPIN, you have to execute `setfirewall.cmd` again (see chapters 4.5 and 8.9)!
2. The NFS Server is only required for AVANCE and AVANCE-II spectrometers.

10. Installing TOPSPIN license (see chapter 7.2)

11. Configuring of TOPSPIN for spectrometer control (see chapter 8.1.1)

Chapter 4

Installing NFS Server

The NFS Server is only required for AVANCE and AVANCE-II spectrometers.If your PC is used as a datastation, no NFS is needed.Furthermor AVANCE-III spectrometers do not need the NFS Server anymore, the **bootparam** process is not required anymore and can be disabled in the list of services (Click **Start → Control Panel → Administrative Tools;** Double-click **Services**; A window '*Services*' will appear: Select the service: **bootparam**; Right-mouse-click on this service and select **Stop**).

4.1 TOPSPIN NT Toolkit CD

The Bruker BioSpin *TOPSPIN NT Toolkit*-CD (for Windows XP) contains the Hummingbird NFS Server 7.1.

The version of the NFS Server for Windows XP that is currently supported is 7.1. If this is already installed, you can skip this chapter.

The NFS Server is available on the *TOPSPIN NT Toolkit*-CD that can be ordered from Bruker BioSpin, part number H9437W0.

Please contact your sales representative for the price of the NFS Server. Alternatively, you can contact NFS manufacturer Hummingbird [1] for information on how

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1. See www.hummingbird.com

to obtain NFS 7.1 or how to upgrade from an earlier version.

4.2 Preparing for the TOPSPIN NT Toolkit installation

The NFS Server 7.1 (!) is required if your PC controls a spectrometer; it makes the DISKLESS package available for the CCU.

Before you install the NFS Server:

- Click **Start** → **All Programs** → **Accessories** → **Command Prompt**
- Enter `ipconfig /all`

and check if the network is installed. If it is not, install the network as described in chapter 13.

4.3 Installing NFS Server

!

IMPORTANT:

- before installing NFS you must configure TCP/IP (see chapter 13.1)
- If your installation fails with following error message:

```
CreatThisService::Createservice:Error # [997]
```

Your network-adapter has no link to the network. Establish a link to the network or install the

```
NWlink IPX/SPX/NetBIOS Compatible Transport Protocol:
```

a) Click **Start** → **Control Panel** → **Network Connections** → Right-click **Local Area Connection xxx**

b) Click **Properties** → **Install...** → **Protocol** → **Add**

c) The `Select Network Protocol`-menu will appear after some seconds. → Click **NWlink ...** → **OK**

d) After some seconds the Properties-menu will reappear: → Click **Close**

If another version is installed, remove it according to chapter 10.2, reboot the computer and install a newer version.

If you have the Hummingbird NFS Maestro CD be aware of the following. An Evaluation CD, will only work for a limited amount of time. Please check if your

delivery contains another NFS Maestro CD. If it does, this is probably the full version. If it does not, you probably ordered an Evaluation CD. Please use the full version if you have one! Now insert the NFS Maestro CD.

4.3.1 Installing NFS 7.1 from the Bruker BioSpin *TOPSPIN NT Toolkit*-CD

1. Log in as a Local Administrator
2. Insert the CDROM *TOPSPIN NT Toolkit*
3. Double-click the icon **My Computer**
4. A window '*My Computer*' will appear:
   - Double-click the CDROM icon
5. A window showing the contents of the CDROM will appear:
   - Double-click the icon **setupNFS** or **setupNFS.cmd**
6. A window '*Hummingbird Master Setup*' will appear:
   - Click **Install NFS Maestro Server**

     This window will change to the subtitle '*Installation Type*'
     - Click **Personal Installation**
     - A window '*Chose Setup Language*' will appear:
       - Choose **English (USA)** (this description is written for the English one)
       - Click **OK**
     - A window '*Hummingbird Setup Wizard*' will appear and display several progress bars. Finally it shows:

       The Hummingbird Setup Wizard will install Hummingbird NFS Maestro Server on your computer ...
       - Click **Next**
     - A window '*License Agreement*' will appear:
       - Click **I accept ...** → Click **Next**
     - A window '*Customer Information*' will appear. Insert the appropriate information or leave the information unchanged (it is important that this application will be installed for anyone who uses this computer):
       - Click **Next**
     - A window '*Destination Folder*' will appear:
       - Click **Next**

- A window '*Setup Type*' will appear:
    - Click **Typical** → Click **Next**
- A window '*Ready to Install the Program*' will appear:
    - Click **Install**
- A window '*Installing Hummingbird NFS Maestro Server*' will appear showing a progress bar
- A window '*Hummingbird Setup Wizard Completed*' will appear:
    - Click **Finish**
- Back in the window '*Hummingbird Master Setup*':
    - Click **Back** → Click **Exit**

7. Remove the CDROM

The certificate '*Proof of license*' is delivered with each TOPSPIN NT Toolkit CD. It proves that you have an official copy of the Hummingbird NFS Server. Please keep this certificate!

4.4 Configuring the NFS Server for spectrometer control

Before you can configure the NFS Server [1] (described in chapter 6.6) you must first install packages on the TOPSPIN DVD, particularly the DISKLESS package (see chapter 6.4).

4.5 Firewall configuration for the NFS Server

If you have enabled the firewall under Windows XP SP2, you have to configure the firewall for the NFS Server. This can be done automatically during the TOPSPIN installation or later while executing the setfirewall.cmd (<topspin-home>\prog\bin\Utilities\Miscellaneous\setfirewal.cmd) (see chapter 8.9).

Note: If you have installed the NFS Server after the TOPSPIN installation, you have to configure the firewall again!

---

1. The NFS Server is only required for AVANCE and AVANCE-II spectrometers.

Chapter 5

Installing a PDF viewer.

5.1 When do I need a PDF viewer?

A PDF viewer is required for displaying the TOPSPIN Online Help and for parts of the NMR-GUIDE. A PDF viewer is not installed automatically as a part of TOPSPIN. Bruker BioSpin recommends to use the Adobe Acrobat Reader. The Acrobat Reader is available from Adobe as a download:

http://www.adobe.com

The English version of the Acrobat Reader is available as a download under the following address:

http://www.adobe.com/products/acrobat/readstep2.html

Chapter 6

Installing TOPSPIN

6.1 Preparing for the TOPSPIN installation

Before you install TOPSPIN:

1. TOPSPIN can only be installed on a NTFS filesystem, not on a FAT file system. However, you can convert FAT to NTFS as described in chapter 12.1.2.

2. Before you proceed, make sure you are logged in as a Local Administrator. If you are not sure about this, press **Ctrl-Alt-Del** (just as for a logon). The popup screen tells you the current user-id. If you are indeed logged in as a Local Administrator, click **Cancel**. Otherwise click **logoff** and then log on as an Administrator.

3. Click **Start → All Programs → Accessories → Command Prompt**

   enter: `ipconfig /all`

   and check if the local network is configured. If it is not, configure the network as described in chapter 13.

If your PC controls a spectrometer:

1. Click **Start → All Programs**

   and check if you see the entry NFS Maestro. If it does not appear, install NFS Maestro Server as described in chapter 4.3. [1]

2. Click **Start** → **All Programs** → **Accessories** → **Command Prompt**

enter: `ipconfig /all`

and check if the second Ethernet adapter is configured. If it is not, configure it as described in chapter 13.

6.2 NMR SUPERUSER and NMR ADMINSTRATION PASSWORD

TOPSPIN offers password check for the configuration tools of TOPSPIN. During the TOPSPIN installation, you are prompted to define:

1. The username for the so called NMR SUPERUSER. If you choose an NMR SUPERUSER other than Administrator make sure that this user exists. The NMR SUPERUSER can be Administrator (this is the default) or any other user (can also be a Domain account). We recommend installing a special user for this purpose, e.g. a user named *nmrsu* (see chapter 9.1). This user does not need any special permissions under Windows; standard access permissions are sufficient.

- After the installation, the NMR SUPERUSER is the owner of all TOPSPIN program files. Logging in as this user allows you to remove these files, change file permissions etc. The name of the NMR SUPERUSER will be stored in the file: `<TOPSPINHOME>/conf/nmrsuperuser`

2. the NMR ADMINISTRATION PASSWORD to be used for TOPSPIN configuration commands. This password can be freely chosen and is not connected to any user. It is asked for by TOPSPIN commands like `cf`, `expinstall` etc. The encrypted NMR ADMINISTRATION PASSWORD is stored in the file:

`<TOPSPINHOME>/conf/nmradminpassword`

! *Note: The NMR SUPERUSER login password and the NMR ADMINISTRATION PASSWORD have different purposes and are totally independent. Changing one of them does not affect the other.*

With the information about the NMR ADMINISTRATION PASSWORD and NMR SUPERUSER TOPSPIN is ready to be configured. The NMR ADMINISTRATION PASSWORD will be asked for every time a configuration type com-

---

1. The NFS Server is only required for AVANCE and AVANCE-II spectrometers.

mand is entered. If this password is typed in correctly, the command will be executed independent of which user is logged in the operating system. As a result all newly created configuration files will be owned by the user that was logged in at the time the configuration command was executed. Any other user can modify the configuration during his login session, just by knowing the correct NMR ADMINISTRATION PASSWORD. This is possible because all configuration files are read- and writeable for everybody, but TOPSPIN will not write them without the correct NMR ADMINISTRATION PASSWORD!

TOPSPIN also offers a so-called *Security Mode*. With this feature all configuration files are only read- and writeable for the NMR SUPERUSER.

6.2.1 How to change the NMR ADMINSTRATION PASSWORD

The *installnmr* script can be used to change the NMR ADMINISTRATION PASS-WORD and the NMR SUPERUSER. If it is called with the option '-secure', it changes the permissions in a way, that only the NMR SUPERUSER can execute the configuration commands and the resulting files are readable and writable only for him, all other users have read-only permissions.

To change the NMR ADMINISTRATION PASSWORD, you have to:

1. Login as NMR Superuser or Administrator

2. Double click on the icon **Bruker Utilities** on the desktop. A window `Bruker Utilities` will appear

3. Double click on the command prompt

    Note: It is not possible to use a 'normal' windows command prompt, because in this 'special' command prompt of 'Bruker Utilities' there are several parameters and path entries defined.

4. Type in:

    perl\bin\perl prog\bin\installnmr <TOPSPINHOME> <NMRSUPERUSER>

    If you installed TOPSPIN in the default directory and you want to use the user 'nmrsu' as NMR SUPERUSER, you have to type in

    perl\bin\perl prog\bin\installnmr C:\Bruker\TopSpin nmrsu

5. Enter the old password and new password as requested.

6.2.2 How to define a new NMR ADMINSTRATION PASSWORD

To define a new NMR ADMINISTRATION PASSWORD, for example because you have forgotten it, you have to:

1. Login as the Administrator

2. Open a Windows Command Prompt

3. Delete the file <x>\conf\nmradminpassword

4. Enter:

```
perl\bin\perl prog\bin\installnmr <TOPSPINHOME> <NMRSUPERUSER>
```

5. Enter new password as requested.

6.3 Packages on the TOPSPIN DVD

1. TOPSPIN: Acquisition and processing software

   • TOPSPIN PLOT EDITOR: Object oriented WYSIWYG plot editor [1]

   • GNU TOOLS: System tools required by TOPSPIN [1]

2. ICON-NMR: Icon-driven interface for Routine Spectroscopy and Automation

3. NMR-SIM: Program for numerical simulation of NMR experiments

4. NMR-GLP: Program for 'Good Laboratory Practice' tests (requires separate license)

5. NMR-GUIDE: Web-browser based teaching and training program

6. NMR-DATA: example data sets

7. DISKLESS: Spectrometer CCU operating system

8. AURELIA-AMIX-Viewer: multiple object viewer (requires a separate license)

9. Auremol: nD spectrum analysis (requires separate license)

10. Perch: Shift prediction and Modeling Tools (requires separate license)

11. SBASE: Spectra base for AMIX (requires separate license)

12. FLEXLM: License manager required for starting TOPSPIN programs.

---

1. automatically installed as part of the TOPSPIN package

6.4 Installing TOPSPIN

This chapter describes the installation of the TOPSPIN as a local Administrator, using a local NMR Superuser account. Chapter 13.6 describes additional steps which must be taken if you want to install the TOPSPIN in a Domain.

The main decision you have to make during installation is where do you want to install the new TopSpin version. If you have a previous NMR SUITE or TOPSPIN installation on this PC available, you can either:

!

- install the new version in parallel to the previous one
  (e.g. old in `C:\Bruker\TopSpin1.3` and new in `C:\Bruker\TopSpin2.1`)

  or

- install the new version in the same directory as the previous one
  (e.g. old in `C:\Bruker\TopSpin` and new in `C:\Bruker\TopSpin`)

The installation in parallel has the advantage, that the previous version remains unchanged. After a parallel installation you can start working with the new version and if you want to go back to the previous version for whatever reasons you can just start and reuse it.

The installation of TOPSPIN 2.1 offers an automatic import of your individual configuration of a previous version, so that there is no advantage to install the new version in the same directory as the old one.

1. Log in as a Local Administrator
2. Close ALL WINDOWS on the desktop
3. Insert the DVD 'TOPSPIN *2.1*'.
4. Start of the installation
   - If the automatic start of the DVD is enabled, the window described in the next step appears automatically, go to step 5
   - If this window of the next step does not appear automatically, autorun is probably switched off (see chapter 10.3) or open the Windows Explorer, go to the DVD device and double-click `install.cmd` [1].
5. The windows *Welcome to the TOPSPIN Setup* will appear: → Click **Next**

---

1. Please note that there is also a file called 'install' on the DVD. This file is the installation script for Linux, under Windows you have to click on the file 'install.cmd'

6. A window *Release Letter TOPSPIN* will appear:
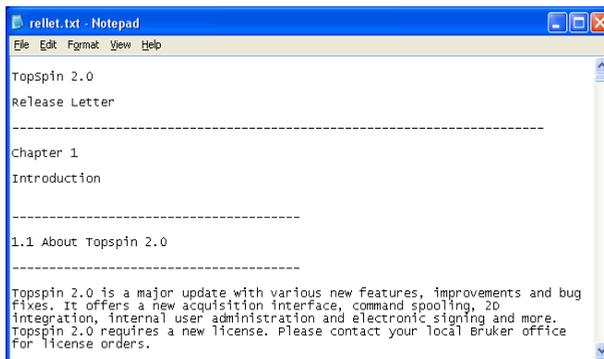
a) Please read the NMR Release letter! You can find therein all information about news and bug fixes of the current version.

b) When you have finished reading the Release Letter, close the Release Letter by clicking the **X** button in the upper right corner.

7. A window *Choose Destination Location* will appear:
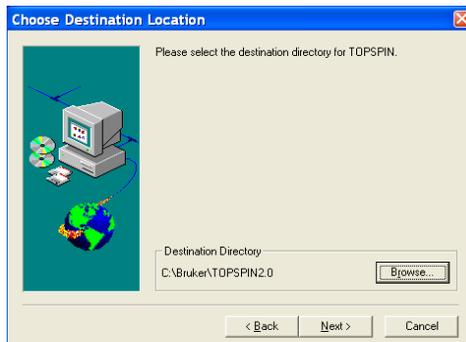
- Select the destination directory for TOPSPIN.

    a) Accept the default destination

    b)   or browse to another destination.
        Enter an installation path which does not exists so far, e. g.
        C:\Bruker\topspin2.1

        - or browse to another existing installation path.
        - Click **OK**

- Click **Next**

8. A window *Select the setup type* will appear:
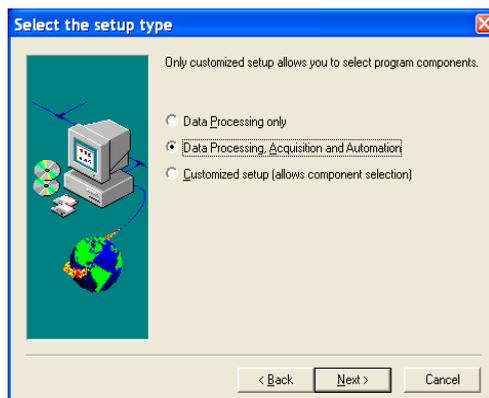
    a) Select the setup type. Do one of the following:

        - Select *Data Processing, Acquisition and Automation* if you want to use
          TOPSPIN for spectrometer control. This will install **Diskless** automati-
          cally.

- Select *Data Processing* if you want to use TOPSPIN for data processing.

- *Customized setup* (allows components selection) if you want to install selected programs only. If you have selected the following window will appear:
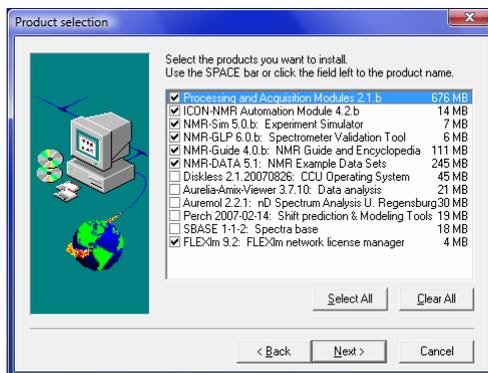
Select the packages which you want to install (note that DISKLESS is only required if your PC controls a spectrometer or you want to configure it e.g. like this:

- TOPSPIN: Acquisition and Processing Modules
- ICON-NMR: Automation Module
- DISKLESS: CCU operating system
- NMR-SIM: Experiment Simulator
- NMR-GUIDE: NMR Guide and Encyclopedia
- NMR-Data: NMR Example Data Sets
- AURELIA-AMIX-Viewer: Viewer of 2D/3D/4D NMR data (requires separate license)
- NMR-GLP: Spectrometer Validation Tool (requires separate license)
- Auremol: nD Spektrum Analysis Tool (requires separate license)
- Perch: Shift prediction & Modeling (requires separate license)

b) Click **Next**

9. A window '*Question*' will appear if Windows XP Service Pack 2 is installed and enabled on your system. If you click *Yes* on the installation configure the

firewall [1] for you.
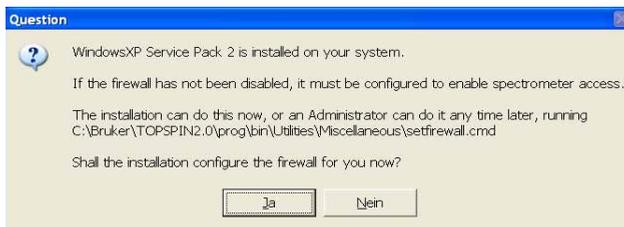
10. A window '*Select Components*' will appear. You can either import no spectrometer configuration, or browse for a spectrometer configuration or select one of the configurations you get offered within this window [2].
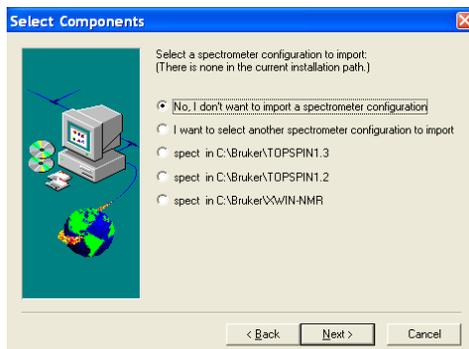
The configurations that are shown in this picture are just an example. On your PC this list could look different.

- Click **Next**

---

1. The firewall must be configured to enable spectrometer access.
2. The installation process will offer all configurations which are available in the Topspin / Xwin-NMR installation that are defined in the registry.

11. A window '*Set NMR Super User*' will appear:

    a) Do one of the following:

- Accept the default NMR Superuser (Administrator) or
- Enter a special user for this purpose, e.g. named *nmrsu* or
- Enter any other user

Under Windows the username must be the name of an existing user. If you choose an NMR Superuser other than Administrator, and this user does not exist yet:

- Press the keys **CTRL+ESC** (to open the Start menu)
- Install a user as described in chapter 9.

    b) Click **Next**

12. A window '*Password Input*' will appear [1] (for more details see chapter 6.2):
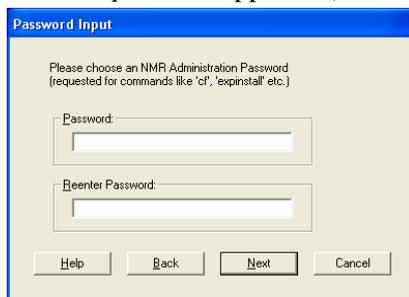
    a) Do one of the following:

---

1. Certain commands like **cf** and **expinstall** ask for the NMR ADMINISTRATION PASS-WORD.

- Type in the NMR ADMINISTRATION PASSWORD
- Re-enter in the NMR ADMINISTRATION PASSWORD

b) Click **Next** → The installation of TOPSPIN will start now.

- destination directory

c) Click **Next**

13. A window '*Setup is complete*' will appear:
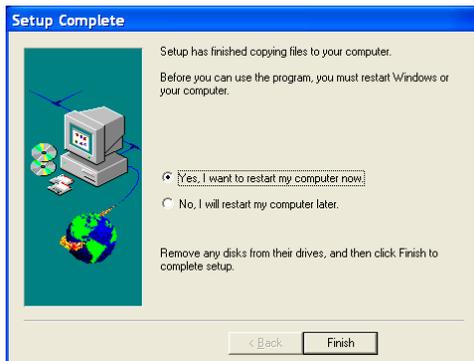
You will be asked if you want to restart the computer:

a) Click **Yes I want to restart my computer now**

b) Click **Finish** (to reboot the computer)

14. After the PC has booted up, press the reset button on the CCU or turn it on with the key if it was switched off. Don't forget to execute '*cf*' and '*expinstall*'!

The following information is for the *Customized setup:*

- It is strongly recommended to accept the default path for the flexLM installation: 'C:\flexlm'! If you choose a user defined path, it may cause some problems with other applications using the FlexLM.

6.5 Installing TOPSPIN patches

Bruker BioSpin recommends installing the latest TOPSPIN patches available.

TOPSPIN patches are parts of TOPSPIN which contain bug fixes. They are available on the Bruker www pages. We recommend to install new patches whenever the *patchlevel* on your system is older than the one on the WWW.

Perform the following steps:

1. Click on the icon **Bruker Utilities** on the desktop.

2. Click **Miscellaneous** → **Patchlevel**
    This will show you the *patchlevel* on your system.

or

3. In TopSpin click **Help** → **Version Info**

    Now check if the Patchlevel on the Bruker BioSpin web server is higher than on your system.

Download from WWW server:

1. Log in on a computer which is connected to the internet

2. Open your web browser

3. Go to *http://www.bruker-biospin.com/software_nmr.html*
    or

4. Go to *http://www.bruker-biospin.com*

5. Click on **Service&Support** → **NMR** → **Software Downloads** and select the operating system and then the package you want to download

6.6 Configuring NFS Server

If your PC is controlling a spectrometer, you must configure NFS after the installation of the DISKLESS package (part of TOPSPIN). This configuration requires that Hummingbird NFS Server is installed (see chapter 4.3). Once this is installed, you can mount any Windows directory from any UNIX host in your network (see chapter 13.4.4). Basically this chapter finishes the installation started in chapter 4.3.

Note: The NFS Server is only required for Bruker AVANCE and Bruker AVANCE-II spectrometers. Bruker AVANCE-III spectrometers do not need the NFS Server.

For this configuration it is very important to turn the Simple File Sharing off:

1. Double-click **My Computer** on the desktop.

2. Click on **Tools**, select **Folder Options**.

3. Click the **View** tab, and then click to select the **Use Simple File Sharing (recommended)** check box to enable Simple File Sharing (click to clear this check box to disable this feature).

1. Click **Start → All Programs → Accessories → Windows Explorer**

2. Select the directory **<TOPSPINHOME>\Diskless** and click with right mouse button.

3. Select in the upcoming window the entry **Properties**

4. Choose the folder **Security**

5. You should see **Full Control** permissions for **Everyone**. Correct this if necessary in the following way:

    • Click **Add**

    • A window *Select Users, Computers, or Groups* will pop up

    • choose the entry **Everyone** in the list **Names**

    • Click **Add**

    • Click **OK**

    • Enable in the '*Permissions*' column '*Allow*' **Full Control**

    • Click **OK**

    • In most cases especially if your PC controls a spectrometer some error messages could appear. A question if you really want do change the permissions in all the subdirectories of *Diskless* may also occur. You can click *OK* in all these windows

6.6.1 Configuring NFS Server 7.1

If you have NFS Server 7.1, proceed as follows:

1. Create the user

    • '**diskless_user_sys**' (with '*account is disabled*') [1]

    and the groups (with no members)

    • '**diskless_group_root**'

    • '**diskless_group_other**'

    • '**diskless_group_sys**'

---

1. Creation and configuration of the necessary user and groups are most convenient if it is done in the user management tool of the management console and not in the user management of the control panel. For starting the management console click right on 'My computer' and choose 'manage'. A new window appears where you can choose 'local users and groups'.

2. Click **Start → Control Panel**

3. The window '*Control Panel*' will appear:

- Double-click the icon **Hummingbird NFS Server**

4. A window '*NFS Maestro Server*' will appear:

a) Click the **Exported File Systems** tab
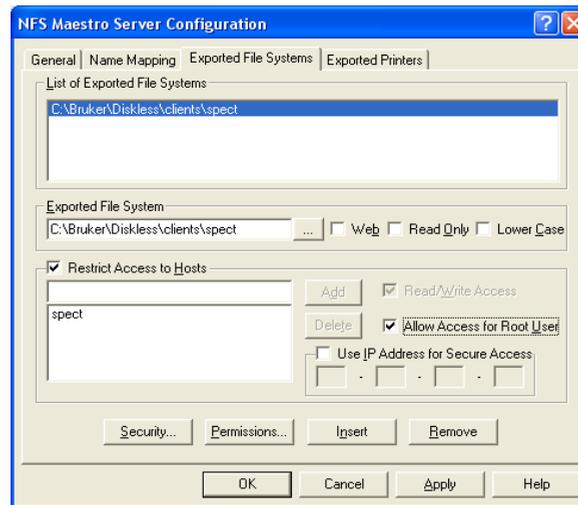
- In the field **Exported File System**: browse for the location of the DISK-LESS package (e.g.: `C:\Bruker\Diskless\clients\spect`)

   Important: the Uppercase letters in this path are necessary!

- Select the **Allow Access for Root User**

- Select **Restrict Access to Hosts**, enter **spect** in the field below and click **Add** → the name spect will appear in the list '*Restricted Access to Hosts*'

- Click **Insert** → 'spect' appears in 'Lists of Exported File Systems'

b) Click the **Name Mapping** tab
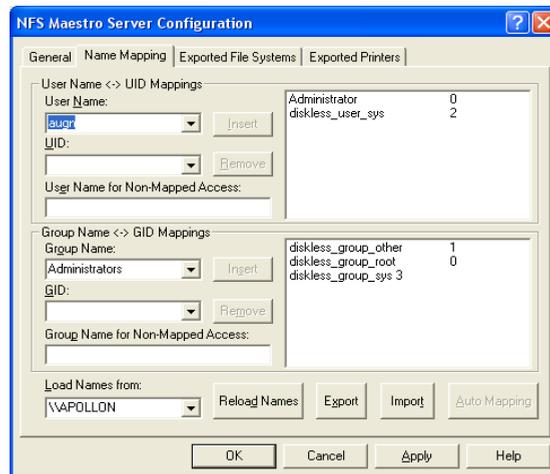
- Click the arrow to the right of the field *Load Names from* and select the local hostname, e.g. **\\MYHOST**

- Click **Reload Names**

- Adding a User mapping
    - In the field *User Name* select the user **Administrator**
        - In the field below, that is called '*UID*' type in '**0**'
        - Click **Insert**
    - In the field *User Name* select **diskless_user_sys**.
        - In the field below, that is called '*UID*' type in '**2**'
        - Click **Insert**

- Adding a Group mapping
    - Select the Group Name using the arrow button in the field below it, type in the GID and click **Insert**
        - Map the group **diskless_group_root** as group with GID 0
        - Map the group **diskless_group_other** as group with GID 1
        - Map the group **diskless_group_sys** as group with GID 3

c) Click the **General** tab

- Click **Server Status**

d) A window '*NFS Maestro Server Status*' will appear:

- Click **Reload Exports**
- Click **OK**

5. In the window '*NFS Maestro Server Configuration*' → Click **OK**

6. If a message about the owner and permissions of spect appears:

- Click **Yes**
- A window '*Permissions*' will appear:
    - Select User: '*Administrator*' and enable Read, Write and Execute permissions for this user
    - Select Group: '*diskless_group_root*' and enable Read, Write and Execute permissions for this group
    - Be sure that also '*other*' has Read, Write and Execute permissions
    - Click **Recursive** → Click **OK**

7. Close the window '*Control Panel*' by clicking the **X** button.

6.7 Adding a user to the group NmrUser

! Every user who wants to run TOPSPIN must be member of the group NmrUser. Adding users to this group is described in chapter 9.1.3.

6.8 Check if the TOPSPIN installation is correct

Double click the TOPSPIN-icon

If you have an valid license you will get this screen:

and TOPSPIN will start.

Unless you already have a license you will get e.g. this screen (for further details

see chapter 7.2):
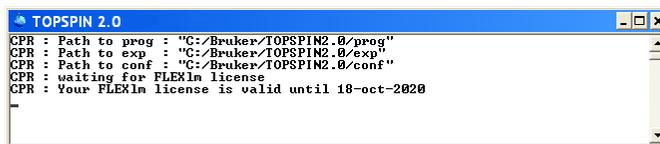
```
TOPSPIN 2.0                                                          _ □ ×
CPR : Path to prog : "C:/Bruker/TOPSPIN2.0/prog"
CPR : Path to exp  : "C:/Bruker/TOPSPIN2.0/exp"
CPR : Path to conf : "C:/Bruker/TOPSPIN2.0/conf"
CPR : waiting for FLEX1m license
lc_set_attr(LM_A_LICENSE_FILE_PTR.003638C0) failed : Cannot find license file
 The license files (or server network addresses) attempted are
 listed below.  Use LM_LICENSE_FILE to use a different license file,
 or contact your software provider for a license file.
License path:  C:\flexlm\Bruker\licenses\license.dat;c:/flexlm/Bruker –
    /licenses/license.dat
FLEX1m error:  -1,212.  System Error: 2 ""
For further information, refer to the FLEX1m End User Manual,
available at "www.macrovision.com".
CPR : No TOPSPIN licence-file installed !
      Please install FLEX1m from the TOPSPIN release CD
      and insert the password in the file "C:\flexlm\Bruker\licenses\license.dat
;c:/flexlm/Bruker/licenses/license.dat"
      according to the TOPSPIN Installation Guide.

      The FLEX1m host ID of this machine is  00040effffff

      If your workstation controls the spectrometer,
      you may run the program without password.
      This requires the acquisition server to be ready.

CPR : checking connection to spectrometer ( may last a minute )
CPR : no spectrometer service license available.

Hit ENTER to continue ... _
```

6.9 Compiling AU programs

TOPSPIN only needs a compiler for the compilation of AU programs. If you do not use AU programs, you do not need a compiler!

TOPSPIN is delivered with the free GNU *gcc* compiler [1].

It is installed automatically during installation of TOPSPIN.

6.9.1 Problems with the default GNU compiler

Generally, the GNU compiler works properly with TOPSPIN. However, if you have a second copy of `cygwin1.dll`, apart from the one delivered with TOPSPIN, you might run into problems. If this happens you will get the following error message:

You have multiple copies of cygwin1.dll on your system.

Search for cygwin1.dll using the Windows Start -> Find/Search facility and delete all but the most recent version. The most recent version *should* reside in x:\cygwin\bin, where 'x' is the drive on which you have installed the cygwin distribution

If you have a problem like this you can remove the second copy of

---

1. If you like to work with the '*vi*' in Bruker's GNU shell, it is necessary to start it with the command '*vim*' in this version of the GNU package.

`cygwin1.dll` (not the one delivered with TOPSPIN).

6.10 The usage of the NMR-GUIDE

NMR-GUIDE 4.1 that comes with TOPSPIN 2.1 uses an own web server and the TOP-SPIN internal java package. Therefore it is not necessary anymore to have these packages installed/configured separately!

6.10.1 Requirements for NMR Guide 4.1

The using of NMR-GUIDE 4.1 requires the installation of TOPSPIN 2.1. Also be sure that the following components are installed:

1. Web browser *Microsoft Internet Explorer*

2. *PDF viewer*

   NMR-GUIDE offers among other things a lot of PDF documents. To display these documents it is necessary to install the acrobat reader. For an installation description see chapter 5.1

3. NMR-GUIDE license (contact license@bruker.de for a three month demo license or order a official license from your local Bruker representative). Note that the NMR-GUIDE license is already part of a full or demo TOPSPIN 2.1 license.

The *Microsoft Internet Explorer* is an official part of the operating system *Microsoft Windows XP*. The WWW browser gets documents from the locally installed WWW server. The client - server communication is established over a network socket connection, but the communication partners only use the localhost TCP/IP host identifier. These pages are shown in the right-hand side window of the browser.

The WWW browser also gets dynamically created pages from the localhost. These workstation specific pages are coming from a *gserver*. This is a platform independent Java web server written by Bruker BioSpin and acts as a daemon running on the locally installed JAVA virtual machine. The gserver is included in the NMR Guide&Encyclopedia package. The table of contents is generated dynamically and displayed in the left-hand side window of the browser.

TOPSPIN commands can be invoked from the WWW browser. This process is also managed by the gserver. The gserver is an essential component of the NMR Guide&Encyclopedia and requires an NMR-GUIDE license.

6.10.2 Java Requirements for NMR-GUIDE 4.1

For using NMR-GUIDE 4.1 that comes with the TOPSPIN 2.1 version it is not necessary to install/configure a special Java package. NMR-GUIDE uses the TOPSPIN internal Java package that is automatically installed and configured during installation of TopSpin.

6.10.3 Working with the NMR-GUIDE

In order to work with the NMR-GUIDE, the following procedure must be followed.

- Start up of the NMR-GUIDE

    1. Start TOPSPIN and enter the command: **`ghelp`**

    2. or enter the command (this allows to start a search within NMR-GUIDE:
       `help`

    3. or select from the *Help* pull-down menu of TOPSPIN the entry:
       NMR-GUIDE

    Your standard web browser will automatically starts and shows the page:
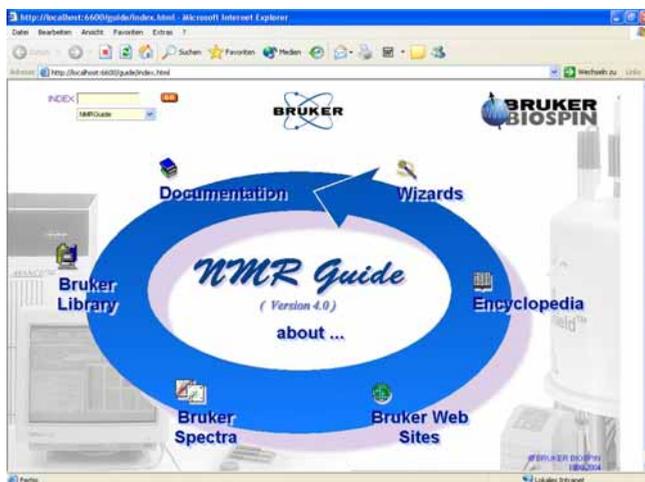
6.10.4 Configuration of Internet Explorer for the NMR-GUIDE

1. Click **Start → All Programs → Internet Explorer**

2. A window *Microsoft Internet Explorer* will appear

3. Click on **Tools → Internet Options → Advanced**

4. Ensure that the following Settings are enabled:

- Java console enabled (requires restart)
- Java logging enabled
- JIT compiler for virtual machine enabled (requires restart)

5. Restart your computer

Chapter 7

The TOPSPIN license

7.1 Questions and answers about the TOPSPIN license

1. *Which programs need a license?*

   TOPSPIN, TOPSPIN PLOT EDITOR, NMR-SIM and NMR-GUIDE need a license. However, if you order a license for TOPSPIN, you automatically get a license for all four programs.

   If you do not have a license for TOPSPIN, it will start up in an emergency mode if your PC is connected to a spectrometer. However, NMR-SIM and NMR-GUIDE will not run without a valid license.

   ICON-NMR is always used in connection with TOPSPIN and does not need an individual license.

   GLP, AMIX, AURELIA, Auremol, MAXENT, PARAVISION and Perch do need a license which must be ordered for each program separately.

2. *Which license types are available and what programs may be run with each?*

   There are six different license types, details of each are given in the following table. For more information please refer to the Bruker license order form in the help menu of TOPSPIN or on the web server:

   https://www.bruker-biospin.com/nmr_license_requests.html

or contact your local Bruker BioSpin representative.

License type	Contents
Full	Acquisition, Processing, Automation (ICON-NMR), Plotting, Experiment Simulation and NMR-GUIDE
	license period: 15 years
	no restrictions
Additional	Acquisition, Processing, Automation (ICON-NMR), Plotting, Experiment Simulation and NMR-GUIDE
	license period: 15 years
	one Full license has to be available
Demo	Acquisition, Processing, Automation (ICON-NMR), Plotting, Simulation and NMR-GUIDE
	license period: 3 months
	Node locked, uncounted, free of charge
Processing-Only	Processing and Plotting
	license period: 15 years
	no Acquisition, no NMR-SIM, no NMR-GUIDE
Presenter	Viewing and Plotting
	license period: 15 years
	no Processing, no NMR-SIM, no NMR-GUIDE
Teaching	NMR-SIM and restricted Processing and Plotting
	license period: 15 years
	TopSpin can only process datasets that are older than 4 weeks or datasets created by NMR-SIM. One TopSpin-plot session (without portfolio editor) can be started, Node locked, count 1.
Developer	Special license for extending TOPSPIN with own functionalities. Allows viewing of data.
	license period: unlimited
	no Processing, no Plotting, no NMR-SIM, no NMR-GUIDE, free of charge

3. *What kind of licenses do I need?*

   If you want to use TOPSPIN 2.x you need a FEATURE line '*TOPSPIN2*' in your
   license.dat file. If you have '*TOPSPIN1*' you can only start TOPSPIN 1.x

and with '*XWINNMR3*' you can only start XWIN-NMR 3.x.

If more than one license is available, as many copies of the program as are covered by the license can be started simultaneously.

4. *Which licensing program is used for TOPSPIN?*

The Flexlm license manager is used and is delivered on the TOPSPIN DVD. The Flexlm package occupies about 3 MByte of disk space. It contains the '*lmgr*' license manager, the '*lmutil*' program, Help files and example `license.dat` file.

5. *What are the requirements for the Flexlm to function:*

- your PC must have an Ethernet card
- the network (TCP/IP) must be installed
- the network Service '*NetBIOS Interface*' must be installed

6. *What is a Floating license?*

Floating licenses are licenses that are available for more than one computer in a network. *Floating* licenses are issued based on the Host-ID of one particular computer. This computer becomes the "license server". All computers that can communicate with this "license server" computer can use the licenses managed by this computer. For this to work, the same license file must be installed on all participating computers, including the "license server". The Flexlm license manager software must only run on the "license server" computer.

A *Floating* license can have just one license for a program like TOPSPIN. In such a case, the respective program can be started once on one computer in the network. If more than one license is available, as many copies of the program as are covered by the license can be started simultaneously. For example, if you have a license file with 5 licenses for TOPSPIN, TOPSPIN can be started 5 times from any 5 computers in the network.

The number of licenses is stated in the FEATURE for the respective program.

7. *What is the difference between 1-Server / 3-Server Licenses?*

Floating licenses can be ordered as 1-server or 3-server licenses. In a 1-server license you have only one license server, and in a 3-server license there are three license servers defined in the license file.

- The advantage of a 1-server license is that it is only necessary to have one computer active at a time to make the license available.

- The advantage of a 3-server license is that any of the three license servers can be inactive and the license management is then done by the remaining two servers.

- One requirement for the three license servers is that all of them have TCP/IP active.

- The operating system on the three computers can be the same or can be different (Linux, Windows).

8. *What is a Node Locked license?*

A node-locked license allows you to start the respective program only on the computer with the Host-ID for which that license was generated. Typically, this license form is used for Demo and Teaching licenses. No other computer can use the license in the way described above for floating licenses.

9. *How do I know if my license is* Floating *or* Node Locked*?*

You can recognize this from the syntax of the license FEATURES in the `license.dat` file:

on PC:

`c:\flexlm\bruker\licenses/license.dat`

on Linux:

`/usr/local/flexlm/Bruker/licenses/license.dat`

If the entry '*HOSTID=*' appears after the encrypted password, the license is Node locked and can only be used on the local PC.

FEATURE TOPSPIN2 bruker_ls 0.0 18-oct-2020 3 2B9E60C19A3C2D4F0DFC \
HOSTID=001125323f2b vendor_info=" for hostid(s) : 001125323f2b" ISSUER=...

→ *Node locked* license for three parallel sessions of TOPSPIN that can be started on the local PC

FEATURE TOPSPIN2 bruker_ls 0.0 18-oct-2020 3 2B9E60C19A3C2D4F0DFC \
vendor_info=" for hostid(s) : 001125323f2b" ISSUER=...

→ *Floating* license for three parallel sessions of TOPSPIN that can be started on every PC in the local network

10. *If I have a* Floating *license and I have a dual-boot PC (e.g Windows XP and Linux), can I use the license on both operating systems?*

Yes, the license is based on the physical address of the Ethernet card and not on the operating system. Copy the license file `license.dat` to:

Windows:

`c:\flexlm\Bruker\licenses\license.dat`

Linux:

`/usr/local/flexlm/Bruker/licenses/license.dat`

11. *How can I determine the hostid of my PC?*

See chapter 7.2.1.

12. *How do I install a license (full or demo) on my PC?*

See chapter 7.2.

13. *Does a Demo license require SERVER/DAEMON lines in* `license.dat`*?*

No, a Demo license is *Node Locked* and therefore only requires FEATURE lines. If SERVER and/or DAEMON lines exist, they are ignored.

14. *I have a* Floating *license. Must the file* `license.dat` *be identical on all hosts, server and clients?*

Yes, you can install `license.dat` on the server and then copy it to all clients.

15. Must the Flexlm license manager run on all hosts in the network?

No, it only needs to run on the license server. If the license manager also runs on a license client, this is simply ignored.

16. *Must the Flexlm license manager run on a host with a Demo license?*

No, it only needs to run on the server for *Counted* licenses.

17. *What can I do if TOPSPIN does not start after I installed the license?*

See chapter 15 .

18. *How is it possible that TOPSPIN starts even though I do not have a license?*

If you do not have a license for TOPSPIN, it will start up in an emergency mode if your PC is connected to a spectrometer. Also one TOPSPIN PLOT EDITOR session (without portfolio editor) can be started from within TOPSPIN. However, NMR-SIM and NMR-GUIDE will not run without a valid license.

19. *What can I do if TOPSPIN cannot find the license.dat file?*

a) Open the **Windows Explorer** and go to `<Flexlm_Home>\Bruker\` → Double-click `lmtools.exe`

A window '*LMTOOLS*' appears.
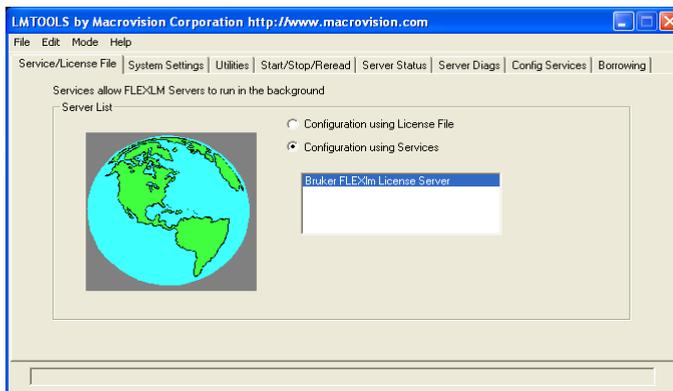
b) Click the **Start/Stop/Reread** tab.
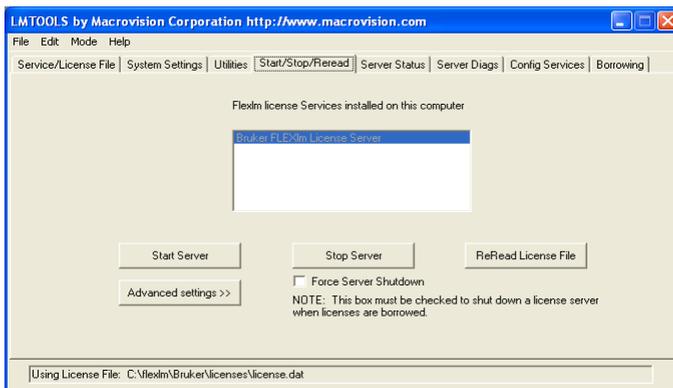
c) Click **Stop Server** → Click **Start Server** → Click **ReRead License file** →
    Click **OK**

d) Close the window '*LMTOOLS*' by clicking the **X** button.

20. *What can I do if TOPSPIN cannot find the license server?*

Please try to restart the license server:

a) Open the Management Console:
    My Computer -> right click **Manage**

b) A window will appear:
    Right click Bruker FLEXlm License Server -> right click **Properties**

c) A window will appear:
If the Service status is 'Started' click *Stop* -> wait and then click *Start* again
If the Service status is 'Stopped' click *Start*

7.2 Ordering and installing the TOPSPIN license

You can order a license from Bruker BioSpin Germany. Demo licenses are free of charge.For licenses you must specify:

- the hostid of your PC (see chapter 7.2.1)

- the program for which you want to get a license, e.g. TOPSPIN

- the type of license (full, demo, processing-only, presentation or teaching)

- the number of licenses and your <u>order number</u> (not necessary for demo license)

Licenses can be ordered from the Bruker BioSpin web pages:

https://www.bruker-biospin.com/nmr_license_requests.html

7.2.1How do I determine the correct hostid

The hostid is a 12-digit hexadecimal number. It is the physical address (also called Mac address or Node address) of the Ethernet card. After installing TOPSPIN, including the Flexlm license manager, you can determine the hostid in two ways:

- Start TOPSPIN; a command prompt will pop up, which will list the hostid, if a correct licence is not yet installed.

- Click the **Bruker Utilities** icon on the desktop, then click **Miscellaneous** → **get_hostid**

- Open a Command Prompt and type in:
  c:\flexlm\Bruker\lmutil lmhostid

  Under Windows XP it is possible to get more than one hostid. Just select one of them to order the license.

Some hostid values may indicate problems:

a) If hostid '*2*' occurs: You may run Windows XP and your network-adapters are disabled.
Click **Start** → **Control Panel** → **Network Connections**

Right-click all **Local Area Connection xxx** -items and there
click **Enable** (if it is visible)

b) If hostid '*0*' or '*ffffffff*' occurs: You may run Windows XP and your net-
work-adapter has no link to the network.

Establish an link to the network or install the

```
NWlink IPX/SPX/NetBIOS Compatible Transport Proto-
col:
```
Click **Start → Control Panel → Network Connections**
Right-click **Local Area Connection xxx**

Click **Properties → Install... → Protocol → Add**
The *Select Network Protocol*-menu will appear after some seconds.
Click **NWlink ... → OK**
After some seconds the Properties-menu will reappear: Click **Close**
See also

```
C:\flexlm\Bruker\help\Index.htm
```

for FlexLM-related problems

7.2.2 Installing a Demo license

A Demo license can be installed as follows:

1. Log in as Administrator

2. Install the Flexlm license manager as described in chapter 6.4.

3. Open a Command Prompt and enter:

- **cd /d c:\flexlm\Bruker\licenses**

- **notepad license.dat**

   enter the FEATURE lines, save and exit the file

You can also install the license file from the Explorer. We have chosen the Com-
mand Prompt because the Explorer might add the (perhaps hidden) extension
.txt to the file license.dat which makes it unusable (see chapter 16.1.3).

7.2.3 Installing a full license on a license server

The Flexlm license manager must always be installed and run as an Windows XP
service on the license server. It is delivered on the TOPSPIN DVD and can be
installed as described in chapter 6.4. The Flexlm is automatically installed as a

Windows XP Service which is then automatically started.

On the license server, the file license.dat must contain a SERVER line, a DAE-MON line and FEATURE lines. An example would be:

```
SERVER petzi 001125323f2b 1700
DAEMON bruker_ls c:\flexlm\Bruker\bruker_ls.exe

FEATURE TOPSPIN2 bruker_ls 0.0 18-oct-2020 3 2B9E60C19A3C2D4F0DFC \
vendor_info=" for hostid(s) : 001125323f2b" ISSUER=0002b39766ed
FEATURE TOPSPIN_1D bruker_ls 0.0 18-oct-2020 3 2B5E00712DB1321F2DDE \
vendor_info=" for hostid(s) : 001125323f2b" ISSUER=0002b39766ed
FEATURE TOPSPIN_2D bruker_ls 0.0 18-oct-2020 3 6B7E009107D129E4DA95 \
vendor_info=" for hostid(s) : 001125323f2b" ISSUER=0002b39766ed
FEATURE XWINPLOT bruker_ls 0.0 18-oct-2020 3 9B5E909100892E5F8A76 \
vendor_info=" for hostid(s) : 001125323f2b" ISSUER=0002b39766ed
FEATURE TOPSPIN_ACQU bruker_ls 0.0 18-oct-2020 3 EBFE503139CA9BE6A280 \
vendor_info=" for hostid(s) : 001125323f2b" ISSUER=0002b39766ed
FEATURE NMRSIM bruker_ls 0.0 18-oct-2020 3 ABFEA0F14EAFD5A666EC \
vendor_info=" for hostid(s) : 001125323f2b" ISSUER=0002b39766ed
FEATURE NMRCHECK bruker_ls 0.0 18-oct-2020 3 7B5ED001633AAAB4D12F \
vendor_info=" for hostid(s) : 001125323f2b" ISSUER=0002b39766ed
FEATURE NMRGUIDE bruker_ls 0.0 18-oct-2020 3 7B7E30D13BDB911F3533 \
vendor_info=" for hostid(s) : 001125323f2b" ISSUER=0002b39766ed
```

where *petzi* is the hostname and *001125323f2b* the hostid of the computer. Note that the second part of the FEATURE lines, the vendor_info, does not necessarily exist. In that case a FEATURE line would look like:

```
FEATURE TOPSPIN2 bruker_ls 0.0 18-oct-2020 3 2B9E60C19A3C2D4F0DFC""
```

To inform Flexlm about the new license proceed as follows:

1. Open the **Windows Explorer** and go to `<Flexlm_Home>\Bruker\` → Double-click `lmtools.exe`

2. A window '*LMTOOLS*' appears. Click the **Start/Stop/Reread** tab → Click **Stop Server** → Click **Start Server** → Click **ReRead License file** → Click **OK**

3. Close the window '*LMTOOLS*' by clicking the **X** button.

7.2.4 Installing a full license on a license client

On a license client, license can be installed in two different ways, as described for a Demo license chapter 7.2.2. The only difference is that you do not have to setup a new file `license.dat`. You can just copy it from the license server which can be another PC (see question 10 in chapter 7.1).

7.2.5 Modifying the license file

To inform Flexlm about the new license proceed as follows:

1. Open the **Windows Explorer** and go to `<Flexlm_Home>\Bruker\` →
Double-click `lmtools.exe`

2. A window '*LMTOOLS*' appears. Click the **Start/Stop/Reread** tab → Click
Stop Server → Click **Start Server** → Click **ReRead License file** → Click **OK**

3. Close the window '*LMTOOLS*' by clicking the **X** button.

7.2.6 Further information

For more information on the Flexlm license manager:

Click **Start** → **run** enter **c:\flexlm\Bruker\help\index.htm** click **OK**

If TOPSPIN does not start after installing the license, please check chapter 15.

Chapter 8

Configuration of TOPSPIN

The idea of this chapter is to give you some guidelines to full spectrometer or workstation configuration. We do not discuss the commands in detail here. For a full description refer to the TOPSPIN manual.

8.1 Configuring TOPSPIN

There are two ways to start TOPSPIN:

1. Click the icon TOPSPIN on the desktop

2. Click **Start → All Programs → Bruker TOPSPIN → TOPSPIN\<vers.\>**

After the first startup of TOPSPIN a window 'License' will appear:

a) Please read the License Agreement for TOPSPIN!

b) When you have finished reading the License Agreement for TOPSPIN and you can confirm the agreement click on **I accept**.

After the window 'License' a window 'configuration check' appears:
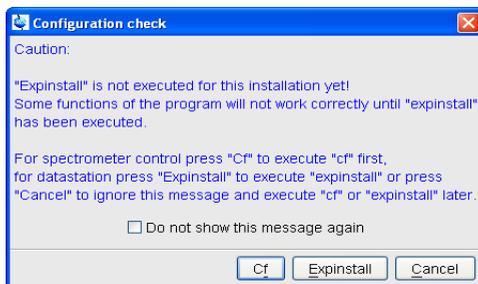
Please configure the software (depends on the hardware of your spectrometer). If you do this, you are mainly in one of the four following situations:

- You have just installed the software in a new directory and the old spectrometer configuration of the software is still known to the new version → go to chapter 8.1.1

- You want to configure a only-processing-PC like your spectrometer-PC, so you have the spectrometer configuration on another computer → go to chapter 8.1.2

- You have to configure the software on a new hard disk without a backup of the spectrometer configuration, so you have no configuration files anymore → go to chapter 8.1.4

- You have a new spectrometer hardware component, so you have no configuration file so far → go to chapter 8.1.5

If you would like to take over the configuration of an existing XWIN-NMR/TOPSPIN into TOPSPIN 2.1 please check chapter 8.2.

8.1.1 If your PC controls a spectrometer:

1. Be sure that the spectrometer is booted (see chapter 6.6 and 15)
2. Open a dataset
   - Type *new* and create a new dataset.
   - You can also select a dataset (e.g. *exam1d_1h*) acquired with another TOPSPIN or XWIN-NMR version.
3. Enter *cf* (The command *cf* now configures the software according to the hardware of your spectrometer):
   a) A window will appear:
      Password request. Please enter the NMR administration password

      Type in the NMR ADMINISTRATION PASSWORD. Click **OK**.
   b) A window will appear:.

Most likely you will select an existing configuration and press "Edit" to confirm this configuration.

c) A window will appear:

The selected configuration is displayed. Choose if would to configure it as a spectrometer or datastation. Choose the type of your spectrometer e.g. **AVANCE** → **ENTER**. Check or type in the 1H frequency of the magnet e. g. **500.13** → **ENTER**. Use the debug mode only in a case of trouble-shooting.
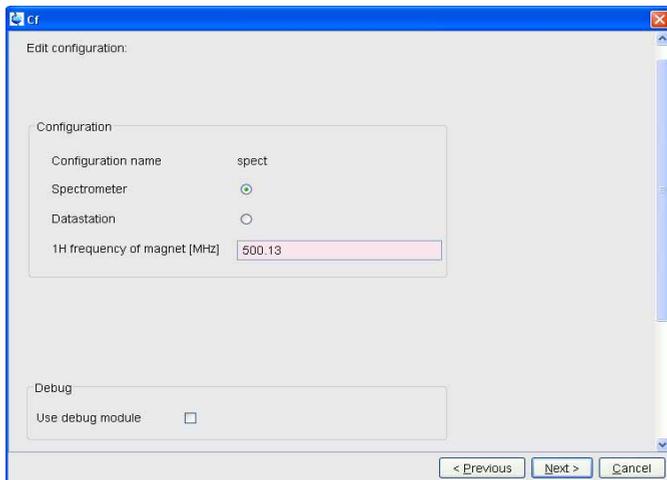
d) If this 'mod hconfserver' information window appears:

- your spectrometer has not a BSMS rack with ECLB board: you may ignore this warning → **ENTER**. Nevertheless please check the Configuration summary (uxnmr.info file) if all units are listed.
- your spectrometer has a BSMS rack with ECLB board: please check if the DHCP server is running. If you are able to start the DHCP server → **ENTER**. If you cannot start the Bruker DHCP service please see chapter 15.6.
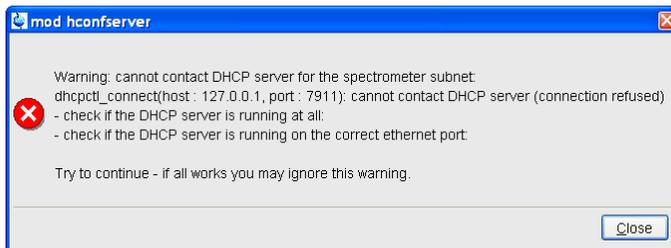
e) A window will appear:
Check if the tty-numbers of the hardware components are set correctly.
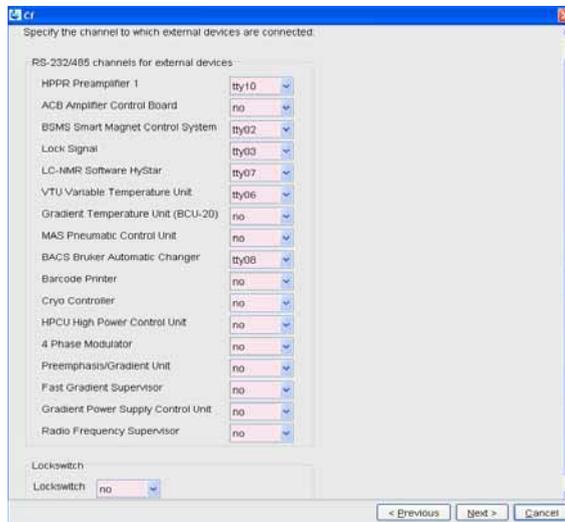
- A window for additional configuration will appear:
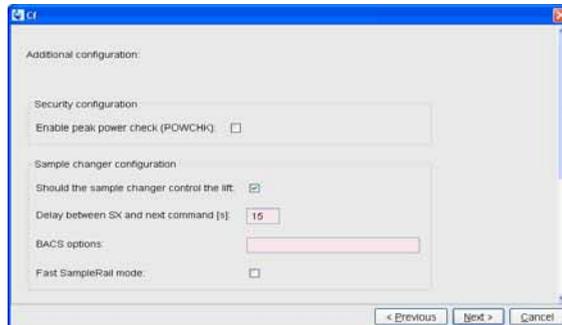
- Choose the option if you need this security options.

  Enable peak power check (POWCHK): (yes/no)

- If you have a sample changer, please select:

  Should the Sample Changer control the Lift: (yes/no)

  The answer depends on how the air flow is connected, normally you will answer: **yes**

  Delay between SX and next command [sec]?

  Type in the length of the delay e. g. **10** → **ENTER**

f) The `nuclei-table` appear.

Check if the frequency of the nuclei are set correctly and click **Save** (If in doubt click **Restore** then click **Save**)

g) A window 'Edit spectrometer configuration will appear:
Check if the preamplifier connections are set correctly and click **Save**..

h) The results of **cf** appears in a text window. Check this list carefully and compare the result with an list from an earlier configuration (if available)

click **Print** and store the paper output with your other spectrometer documentation, then click **Next..**.
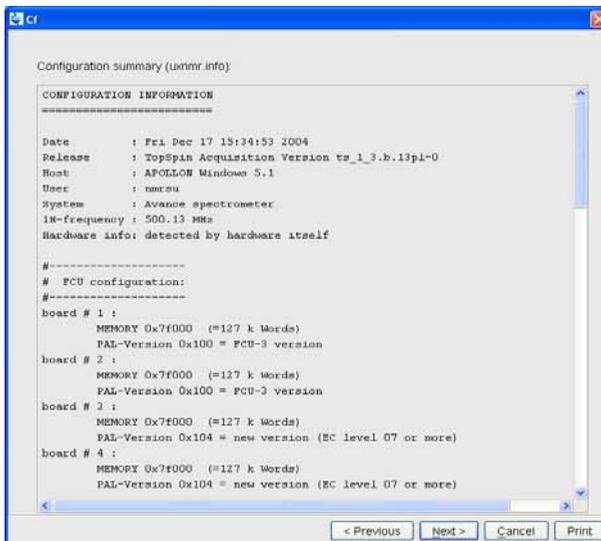
! **If during 'cf' an error message occurs that invites you to do a firmware update see chapter 8.6**

After finishing cf window '*Additional configuration programs*' will appear showing a list of configuration steps. .

Accept the default selection and click on the buttons (You will be asked for the NMR ADMINISTRATION PASSWORD a couple of times):

• Continue with **expinstall**

a) Type in the NMR ADMINISTRATION PASSWORD and **OK**

b) Click **Next** if you either have no modified Bruker BioSpin-Parameterfiles

AU-programs and Pulse-programs or if you have archive them in a different directory. Your individual Parameterfiles, AU-programs and Pulse-programs that have different names to the original Bruker BioSpin files will not be destroyed during the installation

c) In the window that appears → Check *Installation for Spectrometer* → Click *Next*
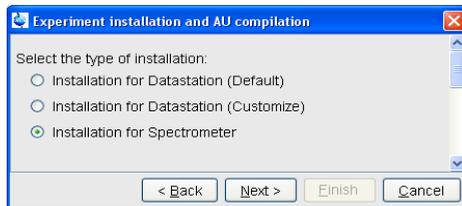
d) In the window that appears → Check e.g. for high resolution NMR *High Resolution Systems* → Click ***Next***
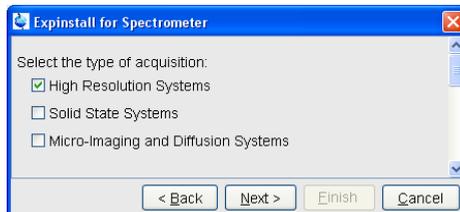
e) In the dialog box that appears → Select the spectrometer configuration name → Click ***Next***
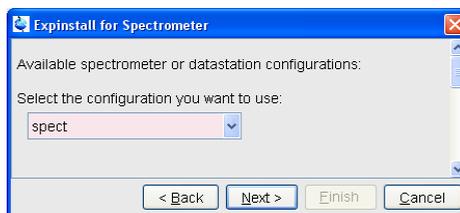
In the dialog box that appears → Check the items you want to install or, accept the default selection → Click ***Next***
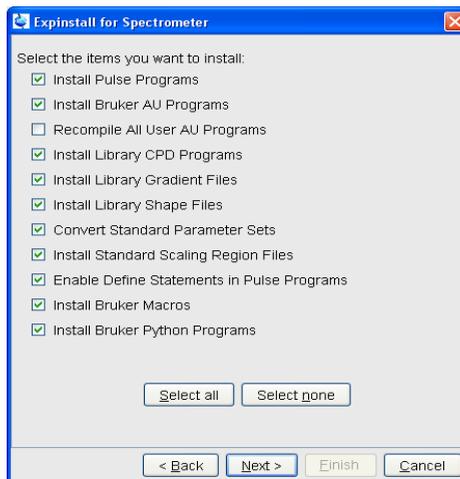
f)   In the dialog box that appears → Select the default printer and plotter and
     the desired paper format → Click **Next**

g)   In the window that appears → Enter the desired spectrometer frequency,
     acquisition mode and pre-scan-delay or, accept the default values
     → Click **Next**
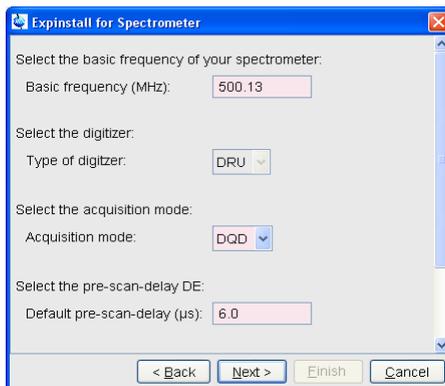
h) In the information box that appears → Check the configuration selection and, if it is correct → Click *Finish*
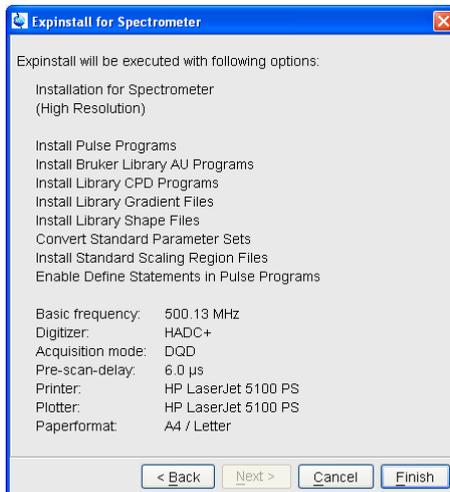
While expinstall will be executed you are able to continue with next configuration program.

- Continue with **edsolv**

Check the list of lock solvents and click **Save** if it is correct → Click **Close**

- Continue with **edhead**
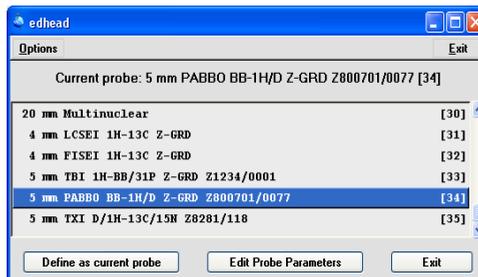
Select the current probe, click the button *Define as current probe* → Click *Exit*
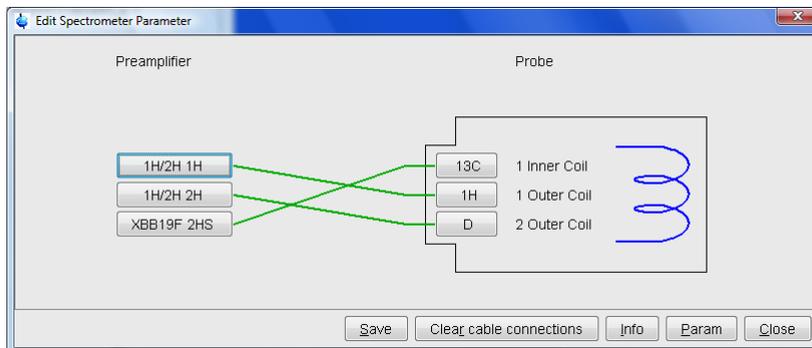
- A window 'Edit Spectrometer Parameter' will appear:

Check if the connections between preamplifier and probe are set correctly →
click *Save* if it is correct → Click *Close*

- Continue with *edprosol*
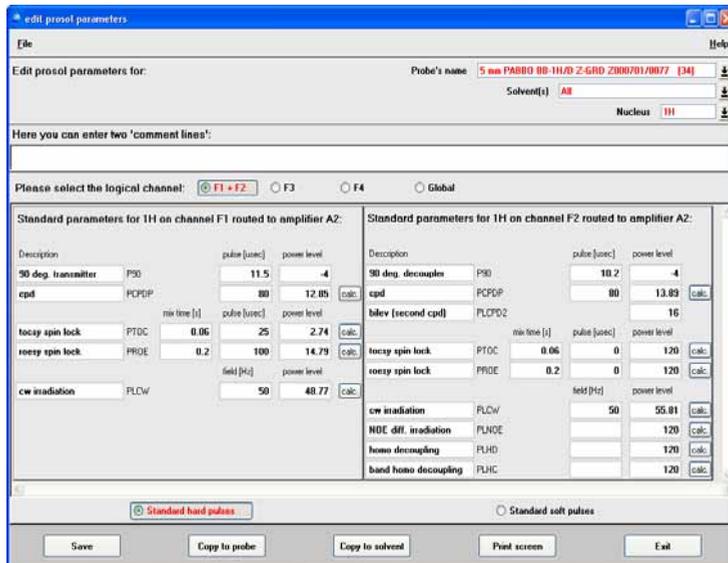
Check the parameters for your favorite nuclei, change them and calculate them,
if necessary → Click *Save* to store to disk → Click *Exit*

- Continue with **`edlock`**
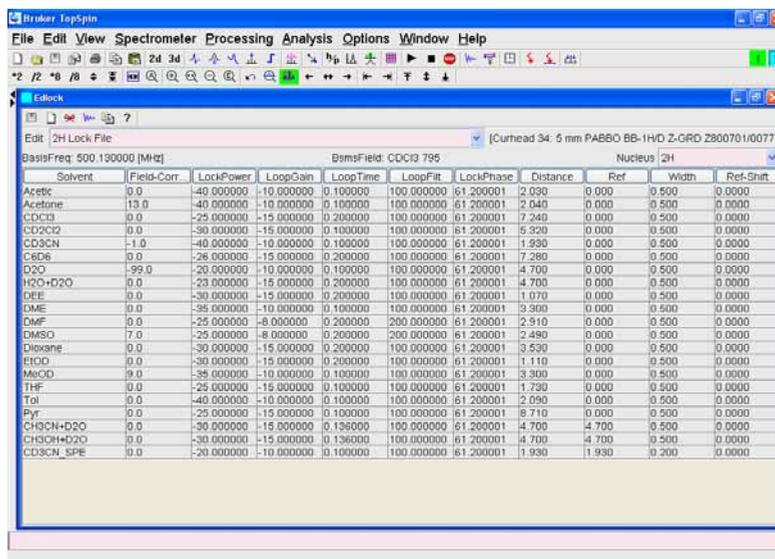
Check the lock table values (field, lock phase, ...), change them. Click **Save**. To close the window, click on the **X** in the right corner.

- Continue with **`edscon`**
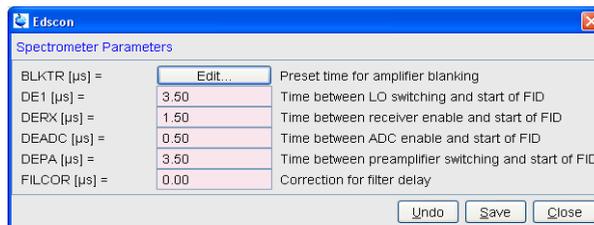
Check the spectrometer constants, change it and click **Save** if necessary, otherwise click **Cancel**

- After finishing the configuration a window `cron check` appears.
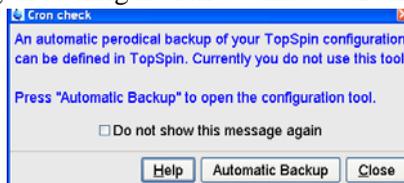
Click on **`Automatic backup`** to set up an periodically backup.
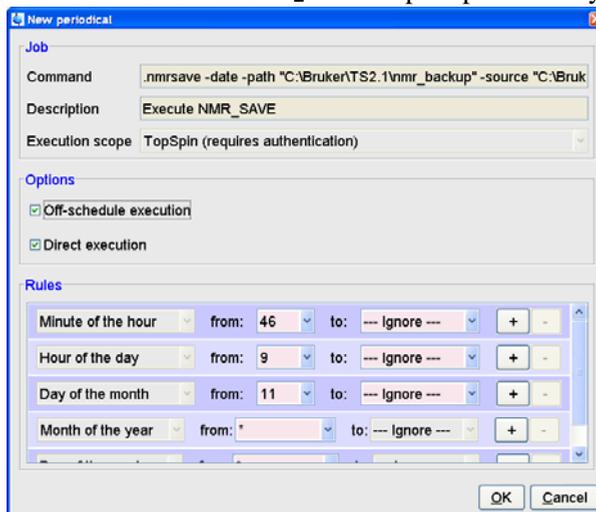
Click **OK** to accept the default. This window (cron command) allows you to executed commands periodically at predefined times. Here you can specify the command to be scheduled, some scheduling options and the starting time and date.

After **`cf, expinstall`**,... have finished insert a sample and make sure that you can lock on the lock solvent. Type **`ii`** and read with **`rpar`** a standard proton parameter file, type **`getprosol`** and **`rga`** and collect a normal ^{1}H NMR spectrum.

8.1.2 If you want to configure a processing-PC like your spectrometer-PC:

If the PC does not control a spectrometer but is used in connection with a particular spectrometer, e.g. for setting up experiments, processing and or plotting, you should configure it as that spectrometer: for example the spectrometer is a AV300 configured with the name 'av300'. Do the following.

a) Copy the configuration directory '`<TOPSPINHOME>/conf/instr /av300`' from the spectrometer AV300 to the workstation.

b) On the workstation paste this '`av300`' directory to '`<TOPSPIN-HOME>/conf/instr`'.

(most likely this is the path: `c:\Bruker\TopSpin\conf\instr`)

You can use the TOPSPIN command **`nmr_save`** to transfer the configuration (see chapter 8.8).

a) Start TOPSPIN as Administrator.

b) Open a dataset

- Type **`new`** and create a new dataset *.*

- You can also select a dataset (e.g. *`exam1d_1h`*) acquired with another TOP-SPIN or XWIN-NMR version.

c) Enter **`cf`** (The command **`cf`** now configures the software according to the hardware of your spectrometer):

    a) A window will appear:

       Password request. Please enter the NMR administration password

       Type in the NMR ADMINISTRATION PASSWORD. Click **OK**.

    b) A window will appear:.
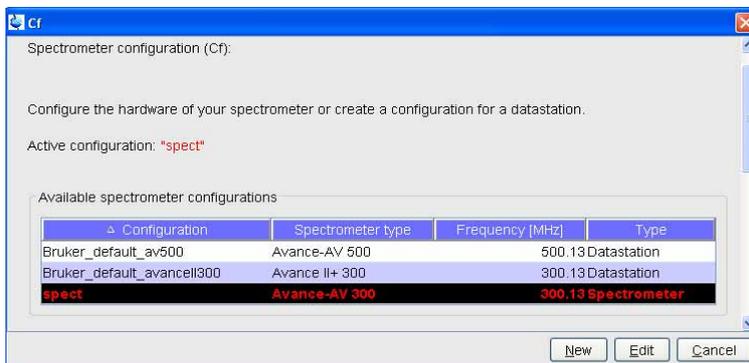
       Press "Edit" to confirm this configuration.

    c) A window will appear:

       The selected configuration is displayed. Choose Datastation to configure

your PC as a datastation.

Edit configuration:

Configuration name   spect

Spectrometer   ○

Datastation   ⦿

Spectrometer type   Avance

1H frequency of magnet [MHz]   300.13

Debug

Use debug module   ☐

< Previous   Next >   Cancel

d) The `nuclei-table` appear.

Edit nuclei table (delete or modify values):
Note: You can also edit this table with the command ednuc
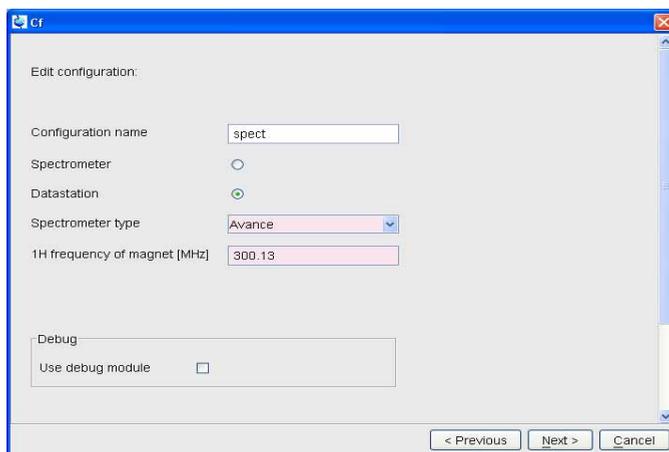
△ Nucleus	Name	Receptivity (rel. 13C)	Spin	Frequency (rel. 1H)
1H	Hydrogen	5680.0	1/2	300.13
2H	Deuterium	0.00821	1	46.071782
3H	Tritium	1.0E-9	1/2	320.130585
3He	Helium	0.00326	1/2	228.637344
6Li	Lithium	3.58	1	44.167389
7Li	Lithium	1540.0	3/2	116.641914
9Be	Beryllium	78.8	3/2	42.173706
10B	Boron	22.1	3	32.244941
11B	Boron	754.0	3/2	96.293631
13C	Carbon	1.0	1/2	75.467749
14N	Nitrogen	5.69	1	21.681046
15N	Nitrogen	0.0219	1/2	30.411909
17O	Oxygen	0.0611	5/2	40.686994
19F	Fluorine	4730.0	1/2	282.404355
21Ne	Neon	0.0359	3/2	23.693151
23Na	Sodium	525.0	3/2	79.390087
25Mg	Magnesium	1.54	5/2	18.372863
27Al	Aluminum	1170.0	5/2	78.204451
29Si	Silicon	2.09	1/2	59.627388
31P	Phosphorus	377.0	1/2	121.494851
33S	Sulfur	0.0973	3/2	23.037979

Add/Edit   Print   Delete   Restore   Save

< Previous   Next >   Cancel

Check if the frequency of the nuclei are set correctly and click **Save** (If in doubt click **Restore** then click **Save**)

e) A window 'Edit spectrometer configuration will appear: click **Save**..
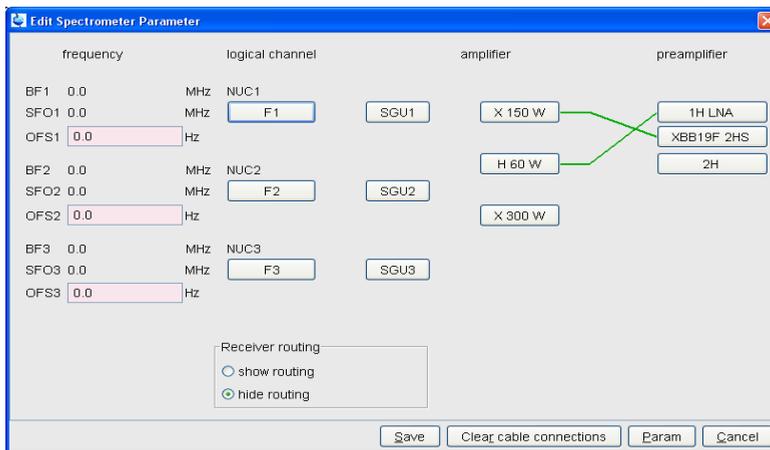
f) The results of **cf** appears in a text window → click **Next..**.

After finishing cf window '*Additional configuration programs*' will appear

showing a list of configuration steps. .

Accept the default selection and click on the buttons (You will be asked for the NMR ADMINISTRATION PASSWORD a couple of times):

• Continue with **`expinstall`**

    a) Type in the NMR ADMINISTRATION PASSWORD and **OK**

b) Click **Next** if you either have no modified Bruker BioSpin-Parameterfiles

AU-programs and Pulse-programs or if you have archive them in a different directory. Your individual Parameterfiles, AU-programs and Pulse-programs that have different names to the original Bruker BioSpin files will not be destroyed during the installation

c) In the appearing window → Check *Installation for Datastation (Customize)* → Click *Next*
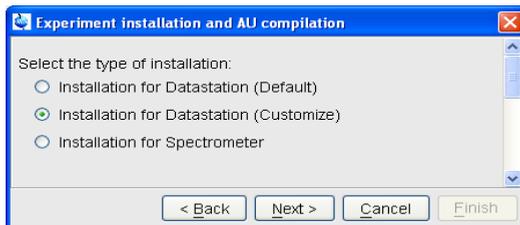
d) In the appearing window → Check *High Resolution Systems* → Click *Next*
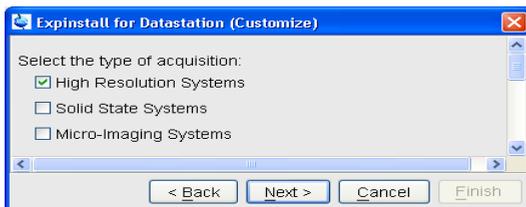
e) In the appearing dialog box → Select the spectrometer configuration name → Click *Next*
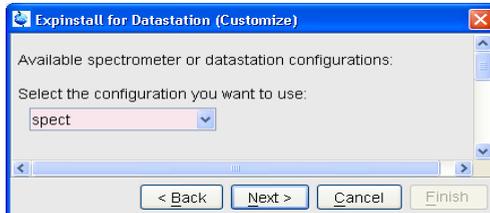
f) In the appearing dialog box → Select the default printer and plotter and the desired paper format → Click *Next*
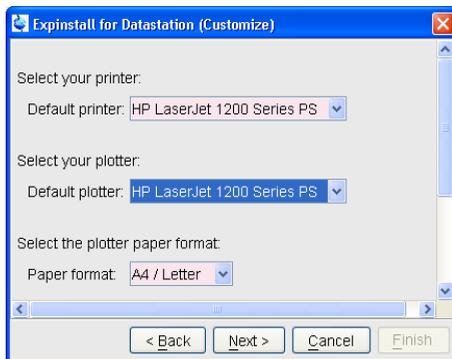
g) In the appearing window → Click *Next*
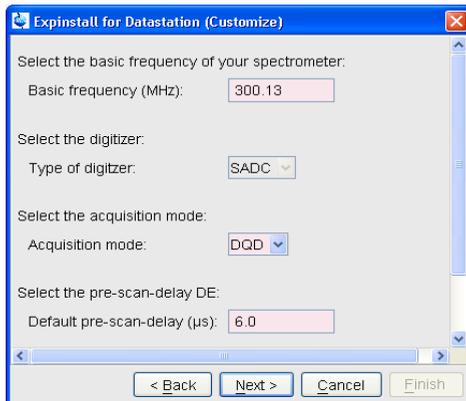
h) In the appearing information box → Check the configuration selection and, if it is correct → Click *Finish*
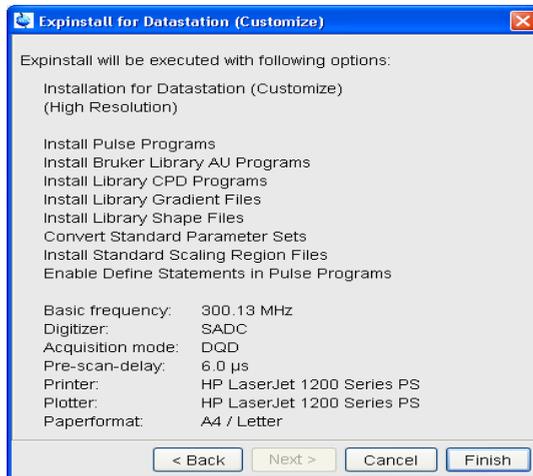
The installation of the selected items, will start now. Wait until this process has finished.

For more details on `expinstall`, please refer to the description of this command in the Acquisition Reference manual.

After finishing the configuration a window `cron check` appears.

Click on **`Automatic backup`** to set up an periodically backup.
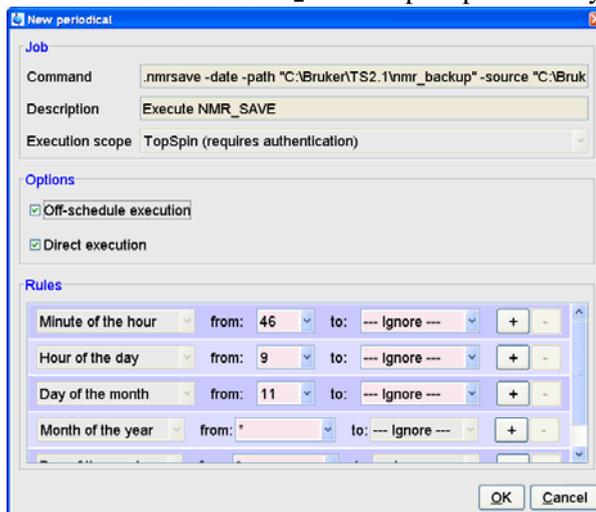
Click *OK* to accept the default. This window (cron command) allows you to ex-
ecuted commands periodically at predefined times. Here you can specify the
command to be scheduled, some scheduling options and the starting time and
date.

8.1.3 If you want to use a default configuration on a datastation

A default configuration can be used on a datastation. It is <u>automatically</u> performed
(no **`cf`** required) during the installation of TOPSPIN on a new computer, a new disk
or in a new TOPSPIN installation directory. The default configuration names are
Bruker_default_av500 (corresponds to an Avance 500 MHz spectrometer) and
Bruker_default_avanceII300 (corresponds to an Avance II 300 MHz spectrome-
ter).

For manual or interactive data processing, the automatic default configuration is
sufficient. If, however, you want to use AU programs, you must execute **`expin-
stall`** once, selecting *Installation for Datastation (Default).*

8.1.4 If you do not know the configuration of your spectrometer

If you do not have any spectrometer configuration information, e. g. after a head-
crash, then you have to recreate the configuration information.

If your spectrometer has a standard configuration, then you can easily do **`cf`** and if

you give the correct information for the '*Type of Spectrometer*' you will get the correct list of your hardware in the '*RS232 table*'. You only have to type in the correct tty's of the interfaces.

8.1.5 If you added a new hardware component to your spectrometer

If you want to add a new hardware component it is recommended to order somebody of your local Bruker BioSpin office to do this for you.

8.2 Take over the configuration of XWIN-NMR or TOPSPIN into TOPSPIN 2.1

The decision how to install TOPSPIN is very important in case you have already XWIN-NMR or TOPSPIN installed on the same or another PC. If so, you might will take over the configuration of XWIN-NMR or TOPSPIN 1.2 / 1.3 / 2.0 into TOPSPIN 2.1 because of:

- in case the XWIN-NMR/TOPSPIN installation was used for controlling a spectrometer there are very important configuration files like the spectrometer configuration, shim files, your own pulse programs, parameter sets, etc.
- if XWIN-NMR/TOPSPIN was used for processing only there can be also very important configuration files like AU programs, macros, plot layouts etc.

! *Note: Transferring files could cause permission problems especially if they are transferred from one PC to another.*

8.2.1 Take over the configuration on the same PC

If TOPSPIN 2.1 is installed parallel to TOPSPIN 1.2 / 1.3 / 2.0 or XWIN-NMR, the AU program **nmr_save** can be used to take over the configuration of XWIN-NMR/TOPSPIN.

You can take over the configuration during the Installation of TOPSPIN 2.1 (see chapter 6.4) or after the installation with the AU program **nmr_save**.

If you like to get more information about the command **nmr_save** refer to chapter 8.8.

Insert the TOPSPIN DVD and start installation. You will be asked to define the installation path. Accept the default or choose another one but not the existing installation directory. During the installation you will be asked if you want to

import a spectrometer configuration. If you want to take over the configuration after installation is finished, start TOPSPIN

- and type in the command:

  nmr_save

- or start TOPSPIN and click

  Options → Manage Configuration → Save installation specific files

A window 'Password request' will appear. Please enter the NMR administration password and click *OK*.

A window 'NMR_Save' appears. Please check the 'Location of Backup file' (default: <TOPSPINHOME>\nmr_backup). Enter the location of the installation to be saved (e.g. C:\Bruker\XWIN-NMR). Click on *Save*.

This will create a tar file of all necessary information from the XWIN-NMR installation. The tar-file is called nmr_backup.tar and will be stored in the directory:

<TOPSPINHOME>\nmr_backup

To take over this information into TOPSPIN, please click on the ***Restore installaton files*** tab, enter the restore destination (e.g. <TOPSPINHOME>) and click on ***Restore***.

After this process is finished, execute ***cf***.

8.3 How to use the Bruker Utilities Folder

After a successful installation of the TOPSPIN, you will find a new folder on every user's desktop named 'Bruker Utilities'. Double click on the folder to see its contents:

or

1. Click **Start → All Programs → Bruker TOPSPIN → Bruker TOPSPIN x.y → Bruker Utilities**

2. A window '*Bruker Utilities*' appears.

In this Utilities folder, you will find commands and applications that you might need when running and configuring a spectrometer. You can see the command prompt right there: just double click on it to get to the prompt.

The other tools are stored in three categories as shown above. You can double click on each of the folders to have them opened up to show their treasures:
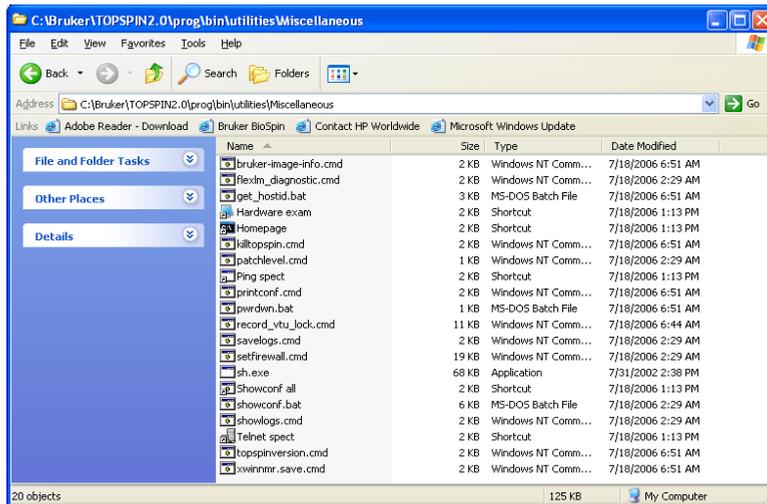
Each of them (our example here is 'miscellaneous') have a number of batches or executables, or plain commands that you can run by just double clicking on the respective icon. For example, to see the system ID of the current PC you can just double-click on the icon called 'get_hostid'. It will open a text window and deliver the system ID you need to know when you apply for TOPSPIN license (encircled):
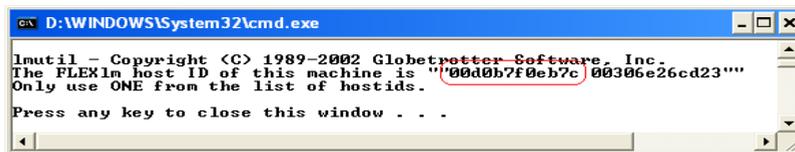
If you press any key, the window will be closed again.

As you can see from the next screen (produced by the command `ipconfig /all` in a command prompt) flexlm takes the address of one of the Ethernet cards in the PC. Which one is used depends on the binding order of the two cards. You

can check the binding by clicking the icon from the Control Panel.

Another interesting tool in the 'miscellaneous' section actually issues commands to the CCU rather than to the PC. One of the items is 'pwrdwn' in this category that logs in to CCU and issues the UNIX command that powers down the CCU. All YOU do is double click on it and watch it do the rest.

The other categories are Service Tools, Test Tools and Documentation. You can just double-click the appropriate icon and the command-shell and tool programs will start up automatically.:
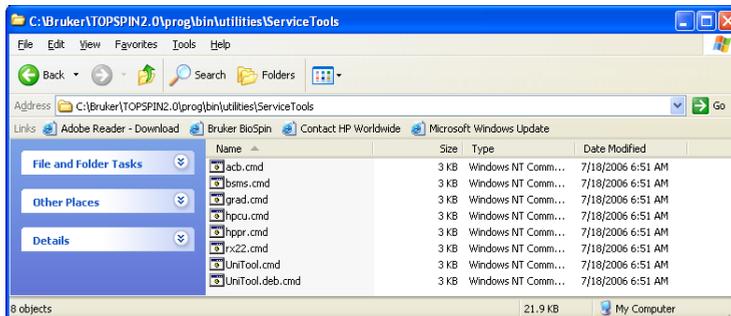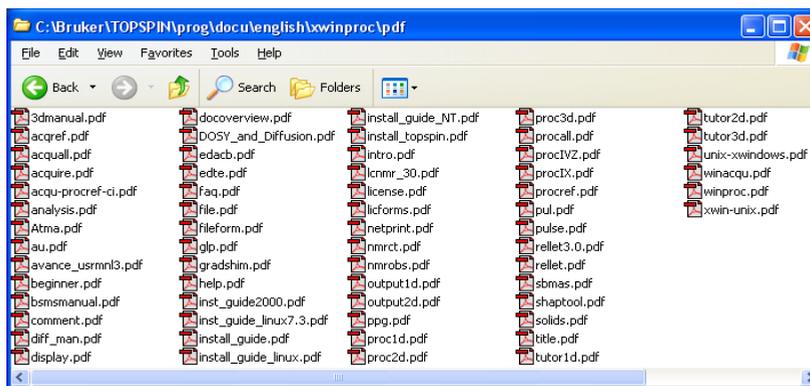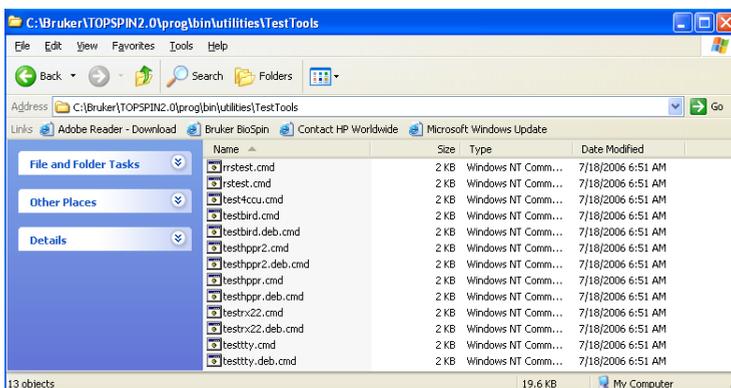
8.4 Configuring the BSMS-Keyboard

For a full description how to configure the BSMS-Keyboard see your

- hard copy of '*BSMS-User Manual*' or
- the respective entry on the '*BASH' CD-ROM*' (Order Number Z36541)

A configuring step that should be done periodically is the spin rate calibration. For this you have to go into the **Menu** mode of your BSMS keyboard. Press simultaneously **2nd** and **Y³**, then rotate the control knob as long as you see **1.Sample** in the display, press **2nd** to go into this directory. The display will show **1.1 Spin calib.** press **2nd** to start this process and wait for ~ 3 minutes.

In this Menu mode, you can also define the helium warning level. If the liquid helium reaches the critical point, the BSMS-Keyboard starts beeping. A special password, the so called security code, is required to be able to change the setting.For an additional possibility to get a warning about a low helium level see chapter 21.1. If in doubt about the setting, contact your service representative.

8.5 How to use the BSMS shuttle

The BSMS shuttle can be used only on spectrometers with BSMS racks with ECLB board.

8.5.1 Requirements

To work with the BSMS shuttle we recommend the following specifications:

- ShuttlePro V.2
- ShuttlePro V.2 software (The following information refers to the ShuttlePro software version 2.0.0)
- TOPSPIN 2.1
- Windows XP Professional SP2
- AVANCE console with BSMS rack with ECLB board

8.5.2 Usage

Standard configuration [1]:

Note: In general it is possible to change these settings under Windows XP [2], but it is not recommended to do this:

a) It is a problem for the service engineer to use the shuttle if everything is configured in a complete different way.

b) There is no support form Bruker BioSpin if the customer has an individual configuration and he runs into problems.

8.5.3 Installation of the BSMS shuttle

1. Log in as a Local Administrator.

2. Connect the ShuttlePro V.2 to an USB port.

3. Close ALL WINDOWS on the desktop.

4. Insert the CD 'Contour Software Installation Disk'.

5. Install the ShuttlePro V.2 (The following information refers to the ShuttlePro V.2 software version 2.0.0).

---

1. This picture is available from the Help menu in BSMS display.
2. It is possible to use your own preferences instead of the standard Bruker configuration. It is only possible to have one configuration for the PC. ShuttlePro V.2 does not support user specific configurations.

Note: The current software version can be downloaded from the web pages of Contour Design Inc..
`http://www.contourdesign.com`

6. After the installation click2.1 right on the ShuttlePro icon close to the time and date in the lower right corner of your screen and choose **Open Control Panel**.

7. The window Contour Shuttle Device configuration will appear.

8. Click on **Options**.

9. Select **Import setting** in the upcoming context menu.

A browser window will appear.

10. Go to your TOPSPIN installation directory into the subdirectory `classes/prop`. In a default configuration this is:
    `C:\Bruker\TOPSPIN\classes\prop`

11. Import the file `TopSpin.pref`.

12. Click on the arrow to select a different Application setting, scroll down and select the entry TOPSPIN.

13. Click on **Options**.

14. Select **Change target application** in the upcoming context menu. A browser window will appear.

15. Go to your TOPSPIN installation directory into the subdirectory `jre/bin` and select the file `java.exe`. In a default installation this is:
`C:\Bruker\TOPSPIN\jre\bin\java.exe`
Now you can enter the TOPSPIN command ***bsmsdisp*** and use the buttons for selecting shims, change values etc.

8.6 Firmware update of the spectrometer hardware

This chapter describes how to update the firmware of spectrometer components. This is only necessary if the cf command has crashed and popped up a message window which informs that you have to do a firmware update of a certain component.

It is strongly recommended to do the firmware update only in this case, because the hardware component could become unusable if the update was done incorrectly.

If you have further questions according firmware updates, please get in contact with your local Bruker BioSpin office. Adresses of several offices can be found in chapter 22, for contact information about all Bruker BioSpin office please go to our web server:

> `http://www.bruker-biospin.de/NMR/about/offices`

8.6.1 Firmware Update for boards without ethernet connection

This chapter describes how to update the firmware for boards without ethernet connection on the example 'LCB board'.

1. Start the '***Service Tools***' of the '***Bruker Utilities***' to check the firmware version of your spectrometer hardware.

2. Double click on an icon starts an automatic procedure that opens a command

prompt. The following example shows the check of the '*bsms-service tool*'

```
C:\WINDOWS\system32\cmd.exe                                    _ □ ×
going to start the service tool "C:\Bruker\TS20b6\conf\instr\servtool\bsmstool\t
ool\bsms.exe" ...
Be sure that the spectrometer is free.
Press CTRL-C to stop or pause




***********************************************************************
***********************************************************************
**                                                                 **
**            ! ! !    W A R N I N G    ! ! !                       **
**                                                                 **
**            This is a hardware level debug tool.                 **
**       Improper operation may damage your hardware.              **
**                                                                 **
**                                                                 **
***********************************************************************
***********************************************************************
*                >>> bsms service toolbox <<<                       *
*                                                                   *
*        Version:          bsms    2.19                             *
*        Compilationdate:  060616                                   *
*        Author:           R.Eggli, M.Schenkel, R.Sauter           *
*                                                                   *
*       Copyright (c) 2004 by Bruker BioSpin AG, Switzerland        *
***********************************************************************


Press Return to abort or 'y' to continue:
```

3. Type **y** → **ENTER**

4. A dialog comes up in the command prompt

```
Select C:\WINDOWS\system32\cmd.exe                            _ □ ×

                  >>>  Main Menu  <<<
0    Keyboard On/Off
1    Init BSMS
2    Check/Download all boards
3    Show all versions
4    Shim functions...
5    BSMS system functions...
6    Board functions CPU...
7    Board functions SCB13R...
8    Board functions SCB7/SCB13M...
9        without SCB13L
A    Board functions SLCB...
B    Board functions LCB...
C    Board functions Keyboard...
D    Board functions GAB...
E    Emulated functions GCB...
F    Service...
Q Quit    ? Help    ! System      Your choice: _
```

5. To check and eventually download a new firmware (from TOPSPIN)

   • type **2**→ **ENTER**

The check starts and ends for example as shown in the following picture

- if there is a problem with a component you get an information to contact your serviceoffice
- if you need a firmware update you will get a message (A) with the length of time for the download (B). It is recommended to do the download as soon as possible.

6. Press **y** → **ENTER** to start the download

! **During the download it is absolutely necessary that spectrometer and PC are not disturbed! Make sure that no one pulls a cable out of the spectrometer or uses Windows XP parallel! (Yes, we know this seems very improbable, but if the download would crash your board might be unusable afterwards)**

- A normal error during downloading the new firmware requires to do the download once again!
- If you have done a download of newer firmware, you have to do **cf** again!
- If you do not need any downloads you can follow the instructions in the command prompt to end this tool.

8.6.2 Firmware Update for boards with ethernet connection

This chapter describes how to update the firmware for boards with ethernet connection on the example 'ELCB board'.

1. To check which ethernet connected hardware units are available you can use one of the two commands **ha** or **ethernet-service-tools**

- Open TOPSPIN and enter in the command line **`ha.`** A window appears that shows several hardware modules.This chapter describes how to update the
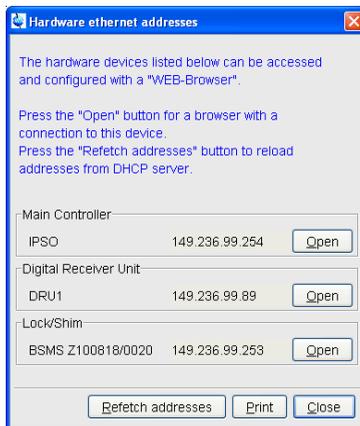
firmware for boards with ethernet connection on the example 'ELCB board'.

- Open **Command Prompt** (Click **Start** → **All Programs** → **Bruker TOP-SPIN** → **Bruker TOPSPIN x.y** → **Bruker Utilities** → **Command Prompt**) and enter the commands:

  - **`cd prog/bin`**
  - Click **Enter**
  - **`ethernet-service-tools`**
  - Click **Enter**

  A window appears that shows several hardware modules.
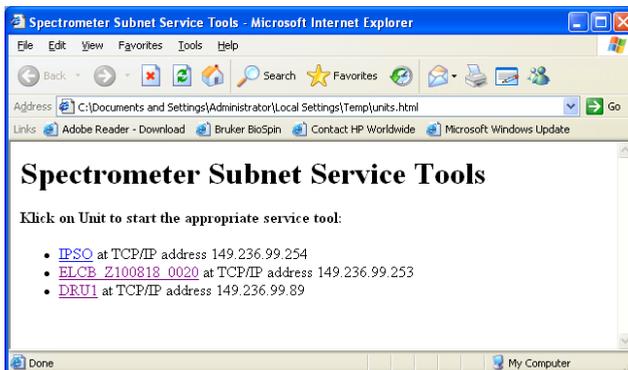
2. Click on the hardware device to open a browser with a connection to this device.

3. A window 'BSMS Service Web - Main' appears. Click on *Device Setup*.
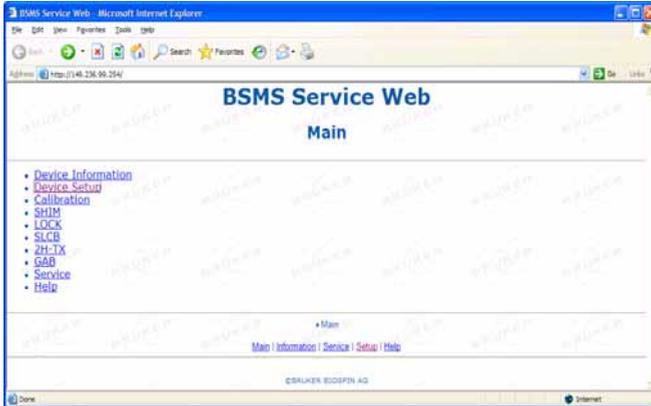
4. The 'BSMS Service Web - Setup' page appears.
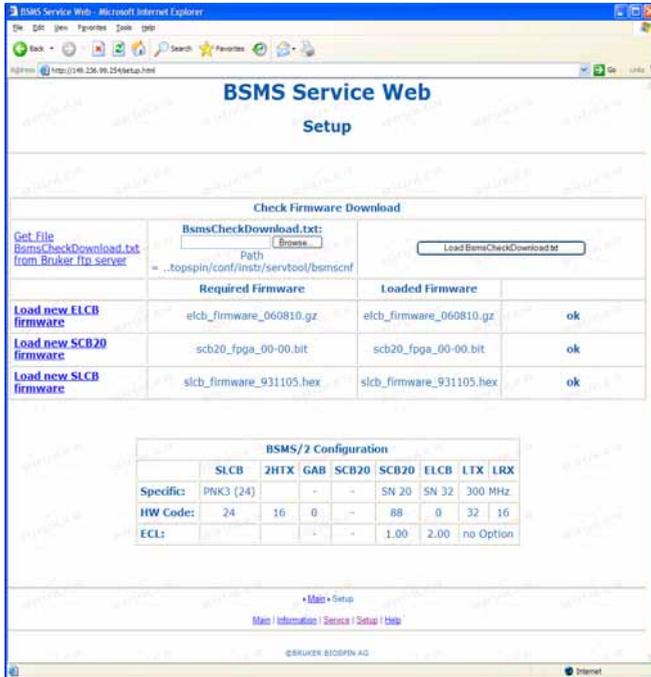
Please click on the button *Browse* to select the BsmsCheckDownload.txt file. In a default installation this file is stored in the directory:

```
C:\Bruker\TOPSPIN\conf\instr\servtool\bsmscnf\
```

*Note: Selecting **Get File BsmsCheckDownload.txt from Bruker ftp server** is only necessary if a Bruker Service Engineer recommends to do this.*

5. After the selection click on the button ***Load BsmsCheckDownload.txt***.

6. If a difference is displayed between *Required Firmware* and *Loaded Firmware* please click on ***Load new ELCB firmware***.

7. The 'BSMS Service Web - ELCB Firmware Download' page appears.
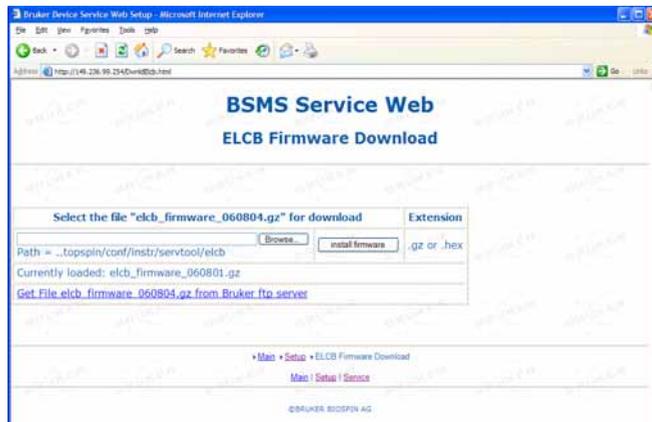
Please click on the button ***Browse*** to select the firmware version which is mentioned in the line *Select the file...*. In a default installation the file is stored in the directory:
```
C:\Bruker\TOPSPIN\conf\instr\servtool\elcb\
```

8. Please click on the button ***install firmware***.

Note: Selecting ***Get File elcb_firmware_XXXXXX.gz from Bruker ftp server*** is only necessary if a Bruker Service Engineer recommends to do this.

Note: The ELCB firmware releases 06xxxx and up are distributed as `*.gz` files. To be able to load this file format to the ELCB the firmware `elcb_firmware_051116.hex` or newer has to be running on the ELCB. If an older firmware is running first download the `elcb_firmware_051116.hex` distribution. The `*.gz` file has to be downloaded as is, don't unzip it!

8.6.2.1 ELCB board: Save user configuration

You can save the user specific configuration of the ELCB board in a Text file.

1. Please open the 'BSMS Service Web' page. Click on *Service*.
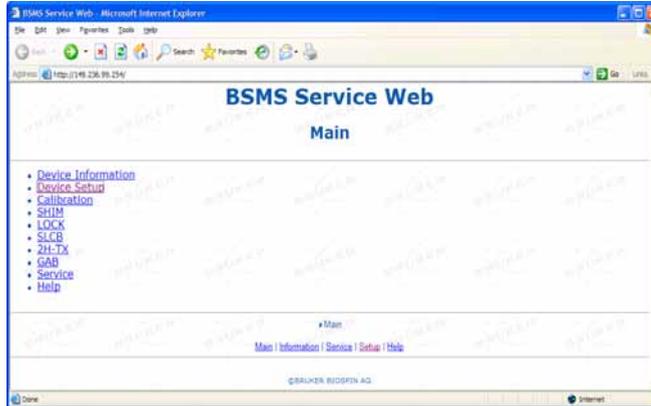
2. The 'ELCB Service Web' page appears. Click under 'Active User Configuration / Parameters' on *Save to Disc*.
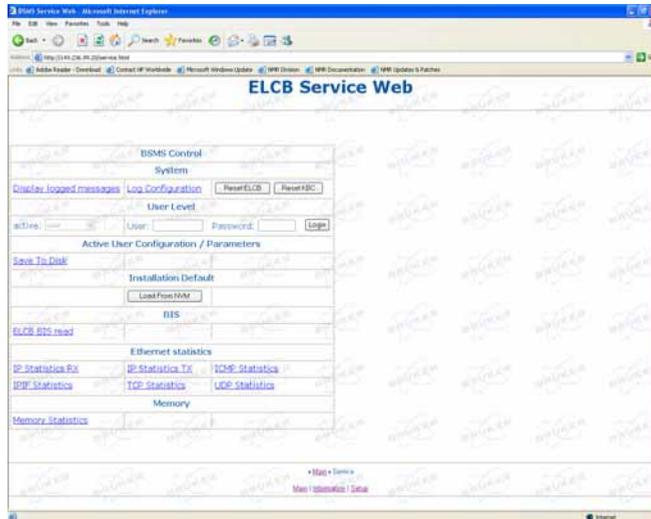
3. The 'BsmsSaveUsrNvm.txt' page appears. Click in the Microsoft Internet Explorer on *File → Save as...* and choose the directory where the file

BsmsSaveUsrNvm.txt should be stored.

8.6.2.2 ELCB board: Restore user configuration

1. Please open the 'BSMS Service Web' page. Click on *Service*.

2. The 'ELCB Service Web' page appears. Click under 'Active User Configura-

tion / Parameters' on *Save to Disc*.
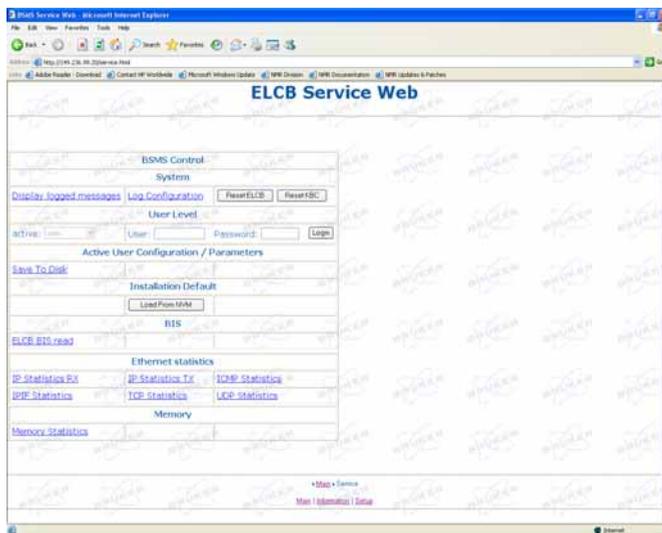
3. The 'ELCB Service Web' page appears. Under 'User Level' you have to enter the *User* and *Password* and click on **Login**.

Note: To get these two information please get in contact with your local Bruker BioSpin office. Adresses of several offices can be found in chapter 22, for contact information about all Bruker BioSpin office please go to our web server:

http://www.bruker-biospin.com/contact_us.html

4. The 'ELCB Service Web' page will be changed. Under 'Active User Configu-

ration / Parameters' click on **Load From Disk**.
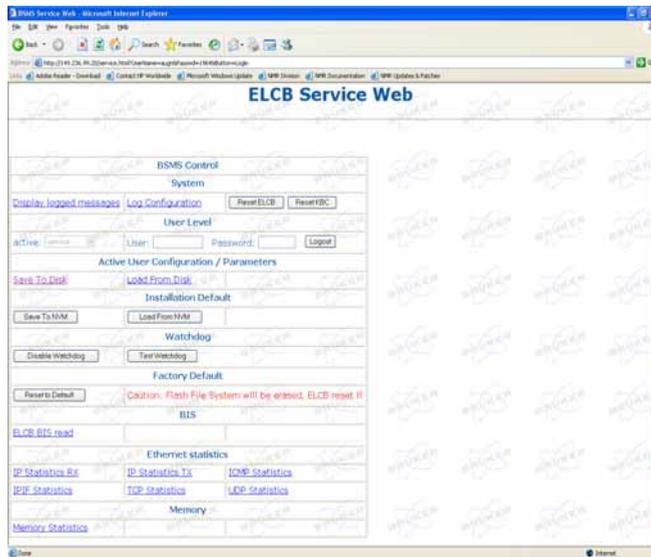
5. The 'BSMS Service Web - Load User Configuration File' appears. Click on **Browse** to select the user configuration file (BsmsSaveUsrNvm.txt) to download. Click on **Submit Query**.

6. The 'BSMS Service Web - Load User Configuration Status' appears. Please check if the 'Status of User Configuration File Load' is 'New User Settings

successfully loaded'.

8.7 A log of the entire system configuration

The *showconf* command provides you with various information about your hardware and software, both of the PC and of the spectrometer. Here is how showconf works: Go to the folder ***Bruker Utilities → Miscellaneous →*** double-click on the ***showconf*** icon and wait about 2 minutes until it has finished. After that showconf has produced a file called confout.txt that contains all you need. Confout.txt is located next to the showconf batch after the first execution and you edit it from there:
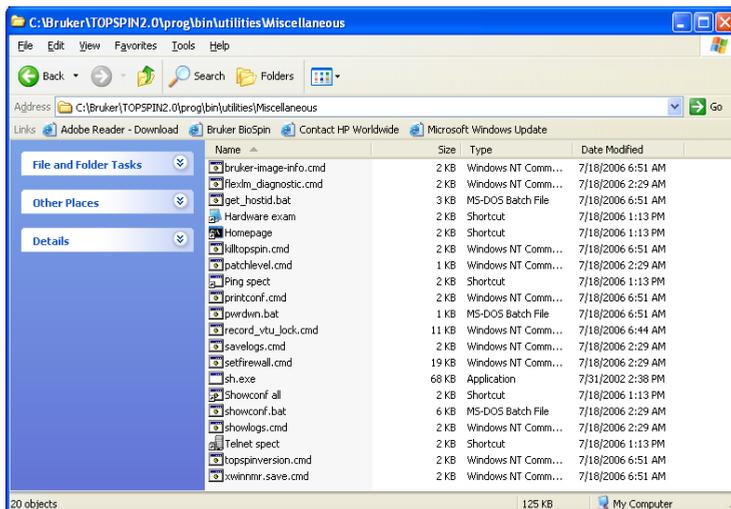
Just double click on the confout icon to call the appropriate editor:

The easiest way to copy it on a diskette is right from within the miscellaneous-folder: Right-click on the `confout`-icon and select 'send to' and then A:
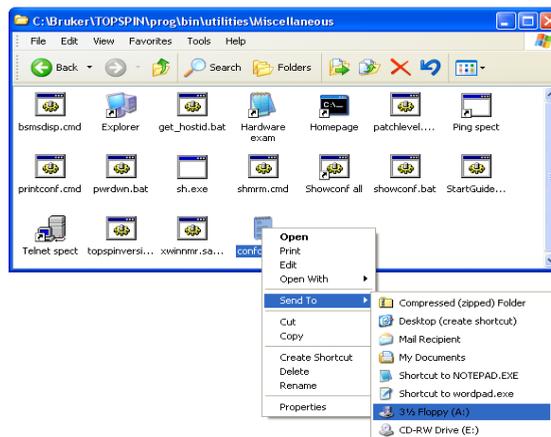
The size of this report is mostly less then 100 kbytes.

DO KEEP A COPY OF THIS FILE IN A SAFE PLACE!

8.8 Backup of VIFs (=Very Important Files) with nmr_save

It is not <u>only</u> necessary to create some backups for the operating system like Boot Disks and to store the acquired datasets.

! it is strictly recommended to create a frequently backup of the 'VIFs' - the 'Very Important Files' of the configuration of TOPSPIN.

There are many reasons like e. g. head crash or theft of the hard disk that makes it important that a weekly or monthly backup is made of important data, so that you would be able to restore the spectrometer configuration in a very short time.

TOPSPIN offers the command[1] (**nmr_save**) for saving those important files that are not delivered by Bruker BioSpin. This command can save and extract user specific data from a TOPSPIN installation and puts them into an archive file.

8.8.1 How to use *nmr_save*

nmr_save can be used for saving and restoring configuration information of the TOPSPIN installation where the command is executed. Furthermore, it is possible to use nmr_save in one TOPSPIN installation to backup data from another TOPSPIN or XWIN-NMR installation.

! In fact, if you have several versions of Bruker software installed in parallel, you should always use the **nmr_save** command from the highest software version.

If your previous TOPSPIN/XWIN-NMR installation is not located on the same PC, you can even mount the respective network path on your local PC and tell **nmr_save** to take over the necessary information over the network.

8.8.2 How to save information with *nmr_save*

nmr_save can be started as follows:

- Start TOPSPIN and type in the command:

  nmr_save

- or start TOPSPIN and click

  Options → Manage Configuration → Save installation specific files

---

1. BRUKER also offers a script (xwinnmr.save) which can be used for saving the 'VIF's (see chapter 21.2).

A window 'NMR_Save' will appear.
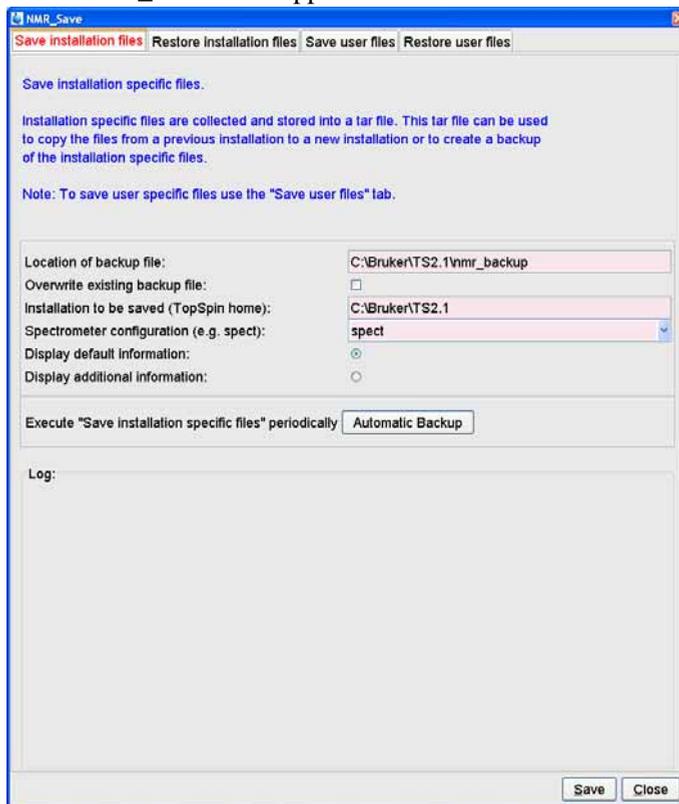
1. Accept or modify the *Location of Backup file*

   (default is: <TOPSPINHOME>\nmr_backup).

2. Enter the location of the *Installation to be saved*

   (default is: <TOPSPINHOME>).

3. **nmr_save** will then offer a list of all available spectrometer configurations which are located in this respective installation. Select the correct configuration in the field *Spectrometer name (spect)*. In a typical setup your spectrometer configuration is called *spect*.

In a typical installation three configuration names will be listed here, your current instrument name and the two Bruker default configurations, *Bruker_default_avanceII300* and *Bruker_default_av500*.

If you are in doubt about the name of your current spectrometer configuration exit the **nmr_save** window and enter the TOPSPIN command **about**. You can find the name of your current configuration in the upcoming window under *Configuration → Current Instrument.*
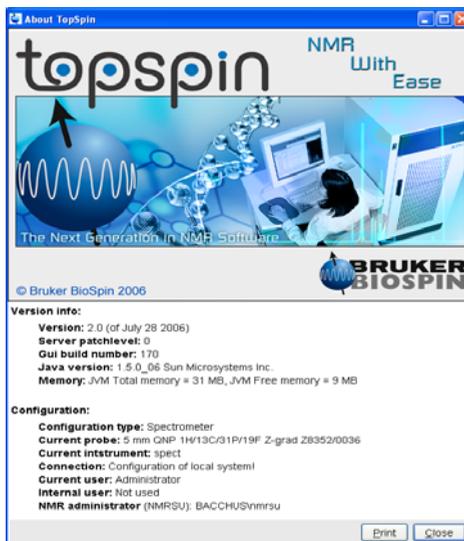
Start **nmr_save** again. Now you can select the correct Spectrometer name.

4. Now you can click on *Save*.

This will create an archive file of all necessary information from the selected installation/spectrometer configuration. This file is called
nmr_backup_<date>-<time>.tar
e.g.: nmr_backup_20071009-2348.tar
and is stored in the directory you selected above, typically:

<TOPSPINHOME>\nmr_backup

If you want to execute 'Save installation specific files' periodically please click on the button *Automatic Backup* this will open a window for a command scheduling. Clicking *OK* will accept the default values and execute **nmr_save** once in a month.
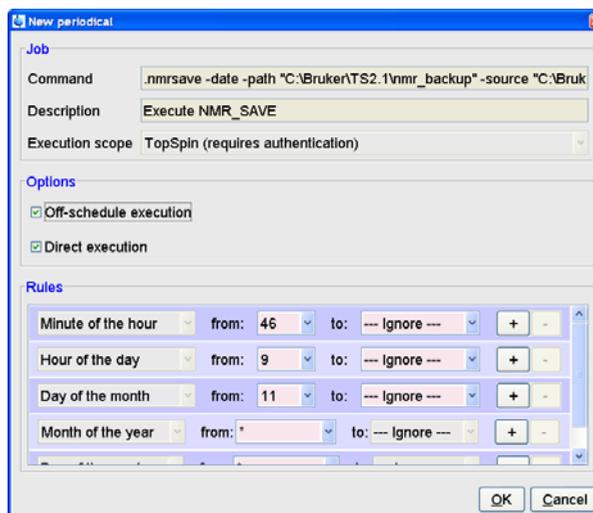
The command cron performs command scheduling. It allows you to executed commands periodically at predefined times. It offers full flexibility in time definition, off-schedule execution and user control. Here you can specify the command to be scheduled, some scheduling options and the starting time and date. The following fields are available:

1. **Command**: The command to be executed.

2. **Description**: A description of the command.

3. **Execution Scope**: The scope of the command execution, User of TOPSPIN. For scope User, the scheduled command will only be executed if TOPSPIN is run by the same (internal) user that is active during cron definition. If the scope is TOPSPIN, the scheduled command will be executed for any (internal) user. Scheduled command with TOPSPIN execution scope can only be defined, cancelled or modified after entering the Administration password.

4. **Off-schedule execution**: This flag allows you to executed commands that were scheduled to run at the time when TOPSPIN was not running. These commands are executed after TOPSPIN startup. Note that commands that were scheduled to run multiple times during Topspin downtime are only executed once.

The following time scheduling rules exist:

- Minute of the hour: 00 through 59

- Hour of the day: 00 through 23
- Day of the month: 00 through 31
- Month of the year: January through december
- Day of the week: Sunday through Saturday

For each of these fields, you can define an interval by selecting a value in the *From* and a value in the *To* field. Setting the *To* field to **Ignore**, schedules the command for execution only at the time/date selected in the From field. An asterix (*) in the From field indicated all possible times. Clicking the + button to the right of a field, adds an extra field of the same type, allowing multiple interval definition. Clicking the **-** button removes the extra field.

8.8.3 Which information is stored with nmr_save?

nmr_save archives some directories completely, in some other directories only specific files. Files that start with an "." are ignored. The internal TOPSPIN database for pulse and cpd programs, macros and python scripts is saved completely. Which information is stored with **nmr_save** can be found below.

The TOPSPIN database is saved completely:

```
<TOPSPINHOME>/db
```

contains pulse and cpd programs, macros and python scripts

The following directories are saved completely (hidden files are ignored!):

```
<TOPSPINHOME>/conf/instr/autoshim/refmaps/
<TOPSPINHOME>/conf/instr/probeheads/
<TOPSPINHOME>/conf/instr/<spect>/prosol/
<TOPSPINHOME>/conf/instr/<spect>/cortab/
<TOPSPINHOME>/conf/instr/<spect>/inmrusers/
<TOPSPINHOME>/conf/instr/topshim/parameters/user
<TOPSPINHOME>/conf/instr/topshim/solvents/user
<TOPSPINHOME>/data/final/nmr/protocolfiles/
<TOPSPINHOME>/exp/stan/nmr/lists/best-nmr/user/subset/fi
<TOPSPINHOME>/exp/stan/nmr/lists/best-nmr/user/subset/lc
<TOPSPINHOME>/exp/stan/nmr/lists/bsms/
<TOPSPINHOME>/exp/stan/nmr/lists/ds/
<TOPSPINHOME>/exp/stan/nmr/lists/eurotherm/corr
```

```
<TOPSPINHOME>/exp/stan/nmr/lists/eurotherm/tcf
<TOPSPINHOME>/exp/stan/nmr/lists/f1/
<TOPSPINHOME>/exp/stan/nmr/lists/group/
<TOPSPINHOME>/exp/stan/nmr/lists/scm/
<TOPSPINHOME>/exp/stan/nmr/lists/vc/
<TOPSPINHOME>/QTP/
```

`<spect>` represents the current spectrometer name or the name specified explicitly when **nmr_save** is started.

From the following directories every file is saved that does not belong to the genuine Bruker BioSpin distribution:

```
<TOPSPINHOME>/conf/instr/servtool/bsmstool/boss
<TOPSPINHOME>/conf/instr/topshim/spect
<TOPSPINHOME>/conf/instr/topshim/probeheads
<TOPSPINHOME>/exp/stan/nmr/lists/gp/
<TOPSPINHOME>/exp/stan/nmr/lists/wave/
<TOPSPINHOME>/exp/stan/nmr/au/scl/
<TOPSPINHOME>/exp/stan/nmr/au/src/
<TOPSPINHOME>/exp/stan/nmr/par/
<TOPSPINHOME>/exp/stan/nmr/parx/preemp
<TOPSPINHOME>/plot/layouts/
<TOPSPINHOME>/prog/tcl/xwish3_scripts/
```

Additionally, the following files are also saved:

```
<TOPSPINHOME>/conf/instr/selpulse.*
<TOPSPINHOME>/conf/instr/probehead
<TOPSPINHOME>/conf/instr/<spect>/2Hlock
<TOPSPINHOME>/conf/instr/<spect>/19Flock
<TOPSPINHOME>/conf/instr/<spect>/best-nmr/CurrPushSolvent
<TOPSPINHOME>/conf/instr/<spect>/best-nmr/hardware.par
<TOPSPINHOME>/conf/instr/<spect>/best-nmr/hardware.src
<TOPSPINHOME>/conf/instr/<spect>/best-nmr/racks.use
<TOPSPINHOME>/conf/instr/<spect>/best-nmr/scanner.src
<TOPSPINHOME>/conf/instr/<spect>/best-nmr/solvents.add
<TOPSPINHOME>/conf/instr/<spect>/best-nmr/solvents.par
```

```
<TOPSPINHOME>/conf/instr/<spect>/best-nmr/solvents.use
<TOPSPINHOME>/conf/instr/<spect>/hardware_list
<TOPSPINHOME>/conf/instr/<spect>/nuclei
<TOPSPINHOME>/conf/instr/<spect>/rs232_device/best
<TOPSPINHOME>/conf/instr/<spect>/rs232_device/bestscan
<TOPSPINHOME>/conf/instr/<spect>/specpar
<TOPSPINHOME>/conf/instr/<spect>/uxnmr.par
<TOPSPINHOME>/conf/instr/<spect>/uxnmr.info
<TOPSPINHOME>/conf/global/layoutsearchpath
<TOPSPINHOME>/exp/stan/nmr/lists/probeheads
<TOPSPINHOME>/exp/stan/nmr/lists/solvents
<TOPSPINHOME>/prog/logfiles/heliumlog
<TOPSPINHOME>/prog/logfiles/heliumlog.err
<TOPSPINHOME>/prog/server/export.conf
<LM_License_File>[1]
```

For safety reasons the tar-file will not be replaced by executing **nmr_save** once again. So if you like to use **nmr_save** several times, you have to move the nmr_backup.tar file from the directory <TOPSPINHOME>/nmr_backup on a backup medium (floppy, CD ...) and then start the script once again or you have to select the 'Overwriting existing backup file' option.

8.8.4 How to restore information with **nmr_restore** (**nmr_save** option)

Note that this will overwrite your complete TOPSPIN configuration plus spectrometer configuration. Restore from a backup file only if you are absolutely sure that this is necessary. If in doubt do not restore or at least create a backup of the current state before.

nmr_restore (**nmr_save** option) offers a field to overwrite an existing configuration. If this is checked the previous configuration is overwritten automatically, if it is not checked, **nmr_restore** will ask you if you are really sure to overwrite the existing configuration

Start TOPSPIN and type in the command:

---

1. This is the environment variable for the license file, in a default installation this is:
    C:\flexlm\Bruker\licenses\license.dat

       `nmr_save`

and click on the *Restore installaton files* tab

or start TOPSPIN and type in the command:

       `nmr_restore`

or click

       Options → Manage Configuration → Restore installation specific files

A window 'NMR_Save' will appear. Select the tab 'Restore installation files'.
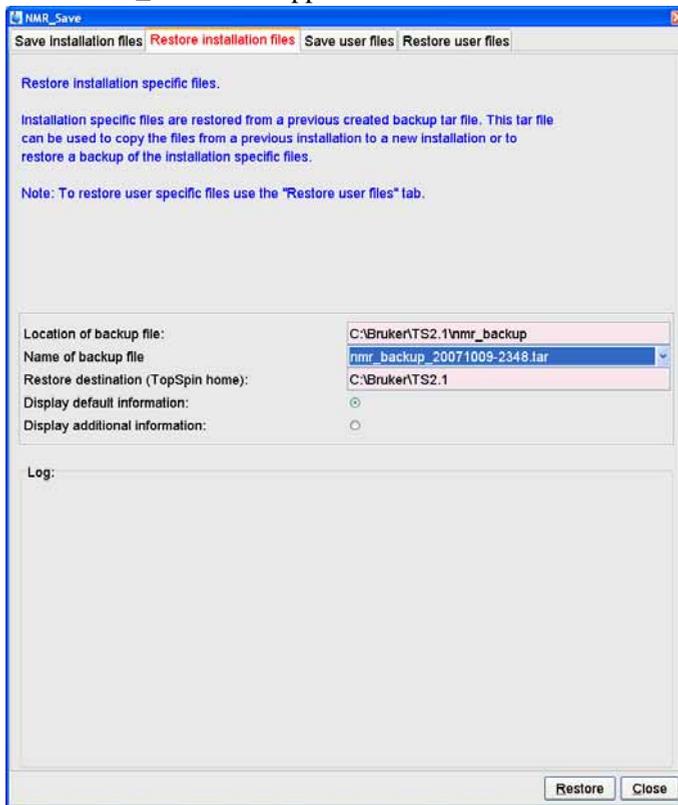
Enter the path where you archive file is stored in the field *Location of Backup file*
(default is: `<topspinhome>\nmr_backup`).

5. Enter the location of the *restore destination*
(default is: `<topspinhome>`)

6. Click on *Restore*

A window 'Password request' will appear.

Please enter the NMR administration password and click *OK*.

7. Execute the TOPSPIN command `cf`

8.8.5 The options for `nmr_save / nmr_restore`

The options for `nmr_save` and `nmr_restore` are:

- `Location of backup file:`
  absolute path where backup archive file `nmr_backup.tar` will be created ('save option') or can be found ('restore option')

- `Overwriting existing backup file:`
  overwrite existing nmr_backup.tar file

- `Installation to be saved or restore destination:`
  a) absolute path to TOPSPIN/XWIN-NMR installation that should be saved.
  b) absolute path where archive file will be extracted.

- `Spectrometer name (spect):`
  name of the spectrometer configuration

- `Display default information`:
  display the directories and files which will be saved

- `Display additional information`:
  display all files which will be saved

8.8.6 Examples for using `nmr_save`

1. Examples for backing up the current TOPSPIN installation:

a) Default backup directory used:

- Location of backup file: `<topsinhome>\nmr_backup`
  (e.g.: `C:\Bruker\TOPSPIN\nmr_backup`)
- Installation to be saved: `<topsinhome>`
  (e.g.: `C:\Bruker\TOPSPIN`)
- Spectrometer name (spect): `<spect>`
  (e.g.: `spect`)
- Click *Save*

b) Default backup directory used, but the spectrometer directory spect_org is saved which is not the default being defined in `<topsinhome>/conf/instr/curinst`

- Location of backup file: `<topsinhome>\nmr_backup`
- Installation to be saved: `<topsinhome>`
- Spectrometer name (spect): spect_org
- Click *Save*

c) /tmp as backup directory:

- Location of backup file: `C:\tmp`
- Installation to be saved or restore destination: `<topsinhome>`
- Spectrometer name (spect): `<spect>`
- Click *Save*

2. Examples for restoring the backup file

a) Restoring the backup file `C:\Bruker\TOPSPIN\nmr_backup\nmr_backup.tar` into the Topspin home directory (default):

- Location of backup file: `C:\Bruker\TOPSPIN\nmr_backup`
- Restore destination: `C:\Bruker\TOPSPIN`
- Spectrometer name (spect): `<spect>`
- Click *Restore*

b) Restoring the backup file `C:\Bruker\TOPSPIN\nmr_backup\nmr_backup.tar` into the directory `C:\Bruker\TOPSPIN\tmp`:

- Location of backup file: `C:\Bruker\TOPSPIN\backup_old`
- Restore destination: `C:\Bruker\TOPSPIN\tmp`
- Spectrometer name (spect): `<spect>`

- Click *Restore*

Note: Do not forget to execute the TOPSPIN command `cf`*.*

8.8.7 How to save information with `user_save` (`nmr_save` option)

`user_save` (`nmr_save` option) can used to copy user specific files to a differnt computer or to create a backup of user specific files of an installation.

`user_save` can be started as follows:

Start TOPSPIN and type in the command:

   `nmr_save`

and click on the *Restore installaton files* tab

or start TOPSPIN and type in the command:

   `user_save`

or click

   Options → Manage Configuration → Save user specific files

A window 'NMR_Save' will appear.
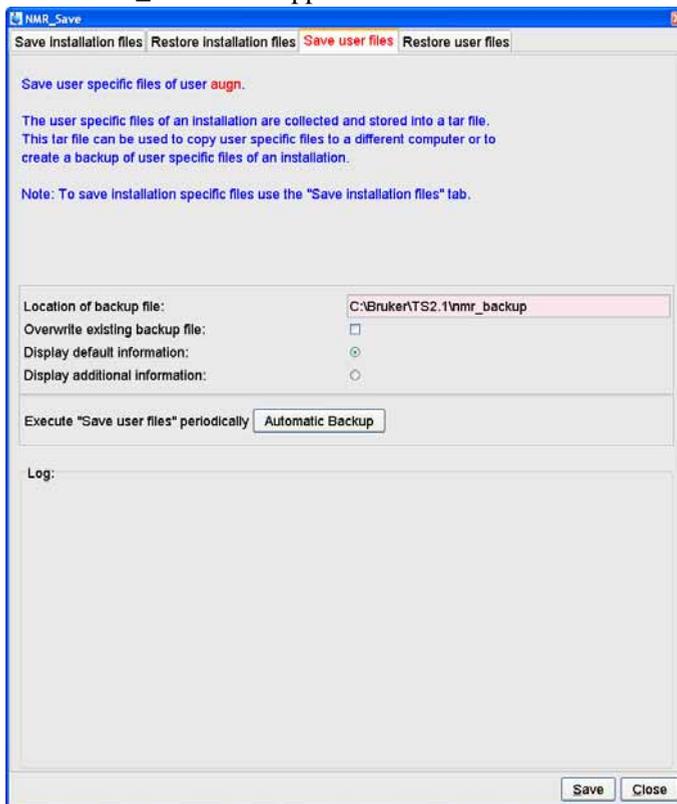
- Accept or modify the *Location of Backup file*
  (default is: `<TOPSPINHOME>\nmr_backup`).

If you want to execute 'Save user files' periodically please click on the button *Automatic Backup* this will open a window for a command scheduling. Clicking *OK* will accept the default values and execute `user_save` once in a month.

8.8.8 How to restore information with `user_restore` (`nmr_save` option)

Note that this will overwrite your user specific files. Restore from a backup file only if you are absolutely sure that this is necessary. If in doubt do not restore or at least create a backup of the current state before.

`user_restore` (`nmr_save` option) offers a field to overwrite an existing

configuration. If this is checked the previous configuration is overwritten automatically, if it is not checked, *user_restore* will ask you if you are really sure to overwrite the existing configuration

Start TOPSPIN and type in the command:

> *nmr_save*

and click on the *Restore installaton files* tab

or start TOPSPIN and type in the command:

> *user_restore*

or click

> *Options → Manage Configuration → Restore installation specific files*

A window 'NMR_Save' will appear. Select the tab 'Restore installation files'.
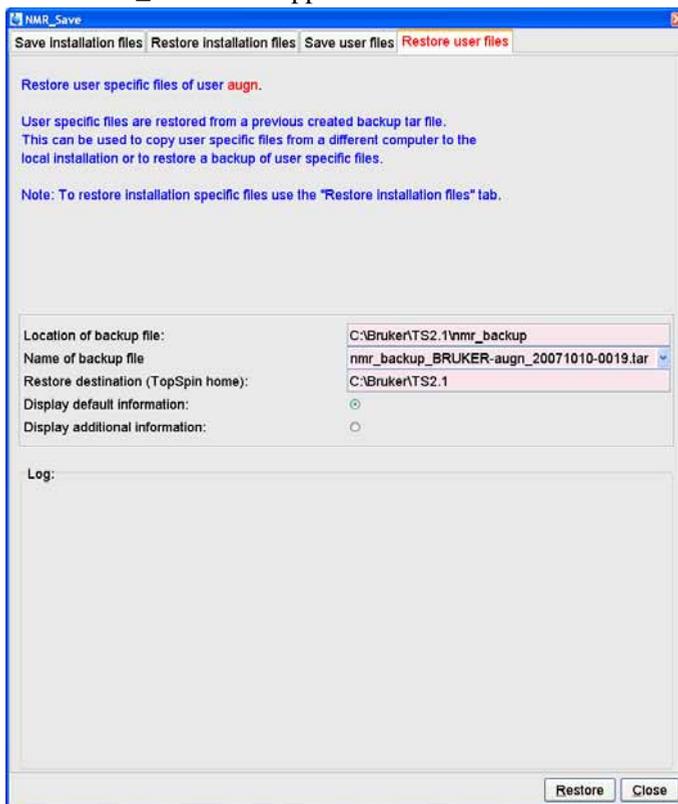
Enter the path where you archive file is stored in the field *Location of Backup file*

(default is: `<topspinhome>\nmr_backup`).

3. Enter the location of the *restore destination*

(default is: `<topspinhome>`)

4. Click on ***Restore***

A window 'Password request' will appear.

Please enter the NMR administration password and click ***OK***.

8.8.9 How to read the archive file

Although the archive file created by **`nmr_save`** is a tar file, it should not be opened or read with the tar command. It is packed in a special procedure and the only correct way of extracting the file is the **`nmr_save`** command!

If you like to have a look at the content of an archive file or copy just some files from it, you should extract the archive into a temporary directory, e. g. `C:\tmp\backup-test`. Then you can check and copy the extracted files from there.

8.8.10 Is all information restored in their original places?

No, the `license.dat` file, the `heliumlog` file and the `heliumlog.err` file are restored in a different directory, because the current ones should not be overwritten. If you want to reuse the restored files you can find them in the restore destination you have chosen, in the subdirectory `<topspinhome>\conf\instr` with the extension `.backup`

All other files are restored in their original places.

8.9 Windows XP SP2 firewall configuration script

Microsoft Windows XP Service Pack 2 (SP2) includes significant changes to Windows networking functionality with regard to security aspects. After installation of

SP2, Windows displays several informational dialogues about 'blocked components' and possible administrators activities during the start-up of TOPSPIN. Bruker BioSpin offers a configuration script 'setfirewall.cmd to apply the required settings to the new Windows XP SP 2 firewall.

Windows now includes fully featured firewall technology ('Windows Firewall', previously known as 'Internet Connection Firewall' or 'ICF'). After installation of SP2, the firewall is activated for all network interfaces by default, blocking network traffic to running applications that is initiated from external network locations. Bruker BioSpin's TopSpin software (as many other applications on the market) makes use of network connections for communication activities. Spectrometer control and TOPSPIN's 'remote connection' feature by design rely on network contacts from outside the local machine. As a result at start of TopSpin, Windows will bring up several information windows about 'blocked programs' recommending an administrator to review firewall settings to allow network communication for designated applications.

It is Microsoft's idea to have Administrators review for which applications network access from outside should be allowed. Those applications should be made 'known' to the firewall thus can be done manually using the '*Windows Firewall*' applet in the Control Panel.

Bruker BioSpin has developed a configuration script '*setfirewall.cmd*' that applies all required settings to Windows firewall configuration without user interaction. The script applies changes to the firewall related to Bruker software only and does not overwrite or reset entries for non-Bruker applications.

The script is stored in the subdirectory `<topspinhome>\prog\bin\utilities\Miscellaneous` of your TopSpin installation.

> *Note: If the script is executed in a wrong directory nothing will happen! Please note that the firewall is configured to allow 'Remote Connection' from local subnet addresses only*

The script can be used in four different ways:

1. During the Installation of TOPSPIN (if the firewall is enabled) you will be asked

to configure the firewall.
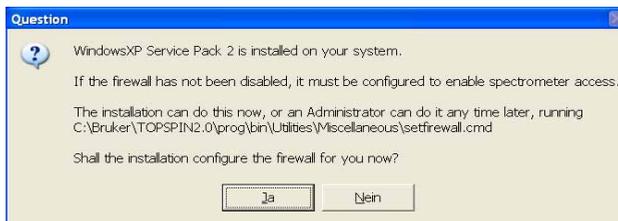
2. Click **Start** → **All Programs** → **Bruker TOPSPIN** → **Bruker TOPSPIN x.y** → **Bruker Utilities** → **Miscellaneous.** Double-click the script file: '*setfirewall.cmd*'. The script will automatically detect the installation path and register this installation with the firewall. I.e., if your installation were in C:\Bruker\TOPSPIN2.1 it would register that and only that!

T

3. Execute the configuration script '*setfirewall.cmd*' from a Command Prompt. You will get usage information like the following:

```
setfirewall INSTDIR SCOPE [DISKLESS_PATH [NFS_PATH]]
```

where

    INSTDIR   installation directory of TOPSPIN, e.g. c:\Bruker\TOPSPIN

    SCOPE   either ALL or SUBNET

                     to specify whether firewall should allow remote connections to this installation from any address or local subnet only.

    DISKLESS_PATH

                     installation directory of DISKLESS, e.g. c:\Bruker\Diskless

    NFS_PATH   installation directory of Hummingbird NFS Server, e.g.

    C:\Program Files\Hummingbird\Connectivity\7.10\NFSServer

Note: You must have administrative rights to do this successfully

This way you have the possibility to register a specific installation of TOPSPIN with the firewall. Example:

```
setfirewall c:\Bruker\ts20 install all
```

would do the required settings for an installation in '*c:\Bruker\ts20*' and allow the remote connection feature to be accessed without restrictions to the initiating network address. You can customize the script for different address ranges if required.

4. Execute the configuration script '*setfirewall.cmd*' from the Bruker BioSpin Command Prompt (e.g. installation in C:\Bruker\TOPSPIN2.1):

- Click **Start → All Programs → Bruker TOPSPIN → Bruker TOPSPIN 2.1 → Bruker Utilities → Command Prompt**

- Enter the command:

  `setfirewall install all`

This way you have the possibility to register the installation of TOPSPIN with the firewall. In this example the configuration script '*setfirewall.cmd*' would do the required settings for an installation in C:\Bruker\TOPSPIN2.1.

In case the installation path of Diskless or the NFS server is different from the default installation path, the script will inform you that the respective firewall configuration entries are not set. You have to execute the script manually and add the correct paths.

In either case, you should consider re execution of the configuration script after one of the following actions happened:

- Complete reset of firewall settings (which is possible e.g. from Control Panel)

- TOPSPIN installation to new location

- Changes in Service Pack status (e.g. reinstallation)

For further questions and contributions, please feel free to contact software support at:

nmr-software-support@bruker-biospin.de

Chapter 9

User Management

9.1 User Management in a standalone PC

After the installation of Windows XP, there is one user with administrator rights, namely the user 'Administrator'. If the password for this user gets lost, there is no way of resetting it other than re-installing Windows XP. Therefore, we strongly recommend you install at least one more user with administrator rights, e.g. with the name 'admin' (actually, this name is also much easier to type on the keyboard).

Now you have for example two users with local Administrator rights, Administrator and admin. Whenever the password of one of them gets lost, you can login as the other one, open the User Manager and define a new password (compare chapter 6.2).

The creation of the new administrator account means that the user 'Administrator' is hidden in the log in menu. You are able to log in as the user 'Administrator' by pressing twice **Ctrl**+**Alt**+**Delete** in the log in window.

You can install a new user or administrator as follows:

9.1.1 Adding a new user in a standalone PC (method 1)

This method is recommended by Bruker BioSpin:

1. Go to the icon **My Computer on the desktop** → right mouse click **Manage**
   or: Open the Microsoft Explorer → Go to **My Computer** → right mouse click
   Manage

2. A window *Computer Management* will appear:
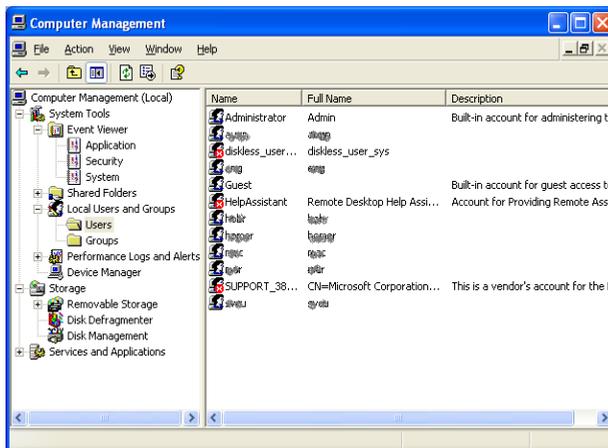
   - Click **Local Users and Groups**

3. Right mouse click **User** → Select **New User**

4. A window '*New User*' will appear

   - Enter the users **Full Name** and **Description** (optional) and the users pass-word in the fields **Password** and **Confirm Password** → **Create** → **Close**

   - If you deselect the option **User must change password at next logon** it is possible to select **User cannot change password** and **Password never expires**.

9.1.2 Adding a new user in a standalone PC (method 2)

This method is not recommended by Bruker BioSpin.

1. Log in as Administrator

2. Click **Start** → **Control Panel** → **User Accounts**

3. A window '*UserAccounts*' will appear:

   - Click **Create a new account**

4. A window '*UserAccounts*' will appear

- Enter the name of the new account e. g. **admin** → **Next**

5. A window '*Pick an account*' will appear

- Click *Computer administrator* → **Create account**

Now you have created a new account. But this account is not protected by a password by default. Therefore you have to set a password for this account!

1. Click **Start** → **Control Panel** → **User Accounts**

2. A window '*UserAccounts*' will appear:

- Click **Change an account**
- Click the account you want to change → Click **Create a password**
- Type in the password, confirm it and type in a password hint → **Create Password**

9.1.3 Adding normal users to the group NmrUser in a standalone PC

Each user who wants to run TOPSPIN must be a member of the group NmrUser. This group is automatically created during the TOPSPIN installation. To add a user, log in as Administrator (otherwise you will be asked for the administrator password during the process) and proceed as follows:

1. Go to the icon **My Computer on the desktop** → right mouse click **Manage** *or:* Open the Microsoft Explorer → Go to **My Computer** → right mouse click **Manage**

2. A window *Computer Management* will appear:

- Click **Local Users and Groups**

3. Click **Groups**

4. Highlight the group '**NmrUser**'

- right mouse click → **Properties**

5. A window '*NmrUser Properties*' will appear:

- Click **Add**

6. A window '*Select Users*' will appear:

- Click **Advanced** → Click **Find Now**
- highlight every name you want to be a member of NmrUsers
- Click **OK** → **OK**

7. Close the window '*NmrUser Properties*' by clicking **OK**

or:

1. Go to the icon **My Computer on the desktop** → right mouse click **Manage**
or: Open the Microsoft Explorer → Go to **My Computer** → right mouse click **Manage**

2. A window *Computer Management* will appear:

- Click **Local Users and Groups**

3. Click **User**

4. Highlight the user '**admin**'

- right mouse click → **Properties**

5. A window '*admin Properties*' will appear. Open the folder *Member of*.

- Click **Add**

6. A window '*Select Groups*' will appear:

- Click **Advanced** → Click **Find Now**
- highlight group you want to be a member of
- Click **OK** → **OK**

7. Close the window '*NmrUser Properties*' by clicking **OK**

9.2 User Management in a Domain PC

9.2.1 Adding a second user with Administrator rights in a domain PC

The group '*domain admins*' are automatically a member of the local group '*administrator*' so it is not necessary to create a second user with administrator rights.

9.2.2 Adding a local user in a domain PC

1. Log in as Administrator

2. Go to the icon **My Computer on the desktop** → right mouse click **Manage**
or: Open the Microsoft Explorer → Go to **My Computer** → right mouse click **Manage**

3. A window *Computer Management* will appear:

- Click **Local Users and Groups**

4. Highlight '*User*'

  - right mouse click → **New User**

5. A window '*New User*' will appear

  - Enter the users **Full Name** and **Description** (optional) and the users password in the fields **Password** and **Confirm Password** → **Create** → **Close**

6. Highlight the user you had just create

  - right mouse click **Properties**

7. A window '*<Username> Properties*' will appear:

  - Click **Member off** → **Add**

8. A window '*Select Groups*' will appear:

  - Click **Advanced** → Click **Find Now**
  - highlight every name you want to be a member of NmrUser
  - Click **OK** → **OK**

9. Close the window '*<Username> Properties*' by clicking **OK**

Click **Start** → **Shut Down**

Select **Log off Administrator**

Click **OK**

Press **CTRL+ALT+DEL**

→ Now you can log on as the new user

9.2.3 Adding normal users to the group NmrUser in a domain PC

Each user who wants to run TOPSPIN must be a member of the group NmrUser. This group is automatically created during the TOPSPIN installation.
To add a user, log in as Administrator (otherwise you will be asked for the administrator password during the process) and proceed as follows:

1. Go to the icon **My Computer on the desktop** → right mouse click **Manage**
   or: Open the Microsoft Explorer → Go to **My Computer** → right mouse click **Manage**

2. A window *Computer Management* will appear:

3. Click **Local Users and Groups**

   • Click **Groups**

4. Highlight the group '*NmrUser*'

   • right mouse click → **Properties**

5. A window '*NmrUser Properties*' will appear:

   • Click **Add**

6. A window '*Select Groups*' will appear:

   • Click **Advanced** → Click **Find Now**

   • highlight every name or group you want to be a member of NmrUser

   • Click **OK** → **OK**

7. Close the window '*<Username> Properties*' by clicking **OK**

9.2.4 Adding a global group to the local group NmrUser in a domain PC

Users who want to use TOPSPIN must be member of the group NmrUser. In a Domain scenario we recommend to administrate users in global groups which are added to the local group NmrUser. Proceed as follows:

1. Go to the icon **My Computer on the desktop** → right mouse click **Manage** *or:* Open the Microsoft Explorer → Go to **My Computer** → right mouse click **Manage**

2. A window *Computer Management* will appear:

3. Click **Local Users and Groups**

   • Click **Groups**

4. Highlight the group '**NmrUser**'

   • right mouse click → **Properties**

5. A window '*NmrUser Properties*' will appear:

   • Click **Add**

6. A window '*Select Users*' will appear:

   • Select in the field '*Location*' the domain name

   • In the window '*Enter Network Password*' type in your login name and password

- Highlight the global group you want to be a member of NmrUsers (normally this is the group '*Domain Users*')

- Click **OK** → **OK**

7. Close the window '*NmrUser Properties*' by clicking **OK**

Part II

Windows XP - Installation and Configuration

Chapter 10

Installation procedure

Before you start:

10.1 Do's and Don'ts under Windows XP

10.1.1 Do not re-install Windows XP

Not only will it usually not cure the problem, you also lose all additional pre-installed software (e.g. TOPSPIN, Office package, user accounting, screen and network drives etc.). YOU will have to put all of these back on manually. In such a case it is very important to have a backup of the essential files (see chapter 15.13 and 8.8). It will be many hours until you are back where you started. **If you have problems, use the Event Viewer and the other diagnostic tools to locate the problem and cure it within Windows XP.** If you think you need a re-install consider an 'Windows XP repair'. Use the Windows XP Repair diskettes (creating described in chapter 12) to repair Windows XP to the status of that repair disk rather than doing a scratch install. Re-installing Windows XP is a last resort and you should have very good reason to do it.

10.1.2 Use Windows sharing rather than FTP

Under Windows you locate other computers in the network with Windows Explorer and then you can use **drag-and-drop multiple files and entire directo-**

ries. You can also connect to UNIX machines in that fashion using a UNIX tool called 'samba'. Installation details are in chapter 13.4.3. Nevertheless, in some cases FTP is still the easiest way to get a file quickly.

10.2 Removing existing software

Windows XP is more complex than you might think. Many files that are uploaded during an installation go into other parts of the system or replace existing versions of files. Thus, an uninstall is more like a build-back and you need that to really clean things out. By removing the directory, you don't solve your problem and also you lose the installation log which is stored as the software is installed. This log is very important and used by the uninstaller to make sure it finds every file that went on in the first place.

Use the uninstaller from Control Panel, i. e. the icon labeled 'Add/Remove Programs'.

Without a log this software will not work any more. If the TOPSPIN is already installed and you want to install a new version or re-install the same version, you must first remove the old version and reboot the computer.

Your own AU programs, pulse programs and parameter sets are NOT removed when you de-install TOPSPIN. If you want to re-install any other package like NFS, you must first remove that package (see below), reboot the computer and then re-install the package.

! Never delete directories to remove a program

Always use the 'Add/Remove Programs' tool

Re-install a program in the following way:

$\rightarrow$ remove the program $\rightarrow$ reboot $\rightarrow$ install the program $\rightarrow$ reboot

1. Click **Start** $\rightarrow$ **Settings** $\rightarrow$ **Control Panel**

2. Double-click the icon **Add/Remove Programs**

3. A window '*Add/Remove Programs*' will appear:

If you want to re-install the entire TOPSPIN (see chapter 6.4), please remove the packages:

- Bruker: TOPSPIN   Bruker: AURELIA/AMIX

- Bruker: ICON-NMR   Bruker: SBASE
- Bruker: DISKLESS   Bruker: FLEXlm
- Bruker: NMR-SIM   Bruker: NMR-GLP
- Bruker: TOPSPIN patches   Bruker: NMR-GUIDE

Note that not all of these packages are necessarily installed!

a) Select the package that you want to remove

b) Click the button **Change/Remove**

c) A window '*Check Setup Information*' will appear

d) Check if the path is correct then click **OK**

e) A window '*Remove Programs From Your Computer*' will appear:

- A growing bar shows the progress of the de-installation
- When the de-installation is finished: click **OK**

f) Repeat step b) to e) to remove further packages or click **OK** to close the window '*Add/Remove Programs*'

4. Close the window '*Control Panel*'

5. Reboot the computer.

During the installation of the TOPSPIN, several entries are made in the Windows XP Registry. If an TOPSPIN package, e.g. TOPSPIN is removed as described above, the corresponding entry in the Registry is automatically deleted.

10.3 Autorun of installation programs

TOPSPIN (like many other software packages) support the Autorun feature. This means that the installation program automatically starts up when you insert the CD-ROM. This, however, only works if the Autorun is enabled. If it is not, nothing will happen after inserting the CD-ROM. In this case you can start the installation program as follows:

1. Click **Start** → **Control Panel**

2. Double-click the icon **Add/Remove Programs**

3. Click **Add New Programs** → **CD or Floppy**

4. A window '`Install Program from Floppy Disk or CD-ROM`' will appear:

The system is looking for a Floppy and/or a CD-ROM. If there are one of these the path will be shown in the field 'Open'

Click **Finish**

4a. If the field 'Open' is empty:

    a) Click **Browse**

    b) In the field 'Look in': select the CD-ROM drive

    c) Find an icon **Setup** or **Setup.exe**

    d) Click **Setup** or **Setup.exe**

or

1. Open the explorer (see 18.1.5)

2. Select the path of the CD-ROM drive (normally D:)

3. Double click on the file setup.exe

The Administrator can re-enable Autorun by changing the Registry entry

!

Warning: You are about to edit the Windows Registry File. This is Windows XP's nerve center and errors in your setup may render your Windows XP installation UNUSABLE. Please make sure you have a recent Windows XP Repair Disk created BEFORE you proceed.

HKEY_LOCAL_MACHINE\SYSTEM\CurrentControlSet\Services\Cdrom\Autorun

from 0 to 1.

Chapter 11

Installing and configuring Windows XP Professional

Windows XP exists in two different forms: Windows XP Professional and Windows XP Home Edition.

The installation as described in this chapter is valid for the English version of Windows XP Professional on a hp workstation xw4400. In this case, you can install Windows XP exactly as described here. For other versions of Windows XP or other hardware, the installation procedure might be different.

For example, on some PC's the boot sequence is interrupted with the **Delete** key rather than with the **F2** key.

This description is intended for new installations. If Windows XP is already installed and you have problems:

!   Before you decide to re-install Windows XP, try to repair

Windows XP

Repairing Windows XP means that you selectively re-install parts of Windows XP, leaving application software and data intact.

11.1 Scratch install of Windows XP

1. If your computer is running:

   a) Click **Start** → **Shut Down** → **Shut down the computer** → **Yes**

   b) When you see the text '`It is safe to turn off your computer`' insert the CD-ROM '*Windows XP Professional*'.

2. Restart the computer and **Interrupt** the boot process by pressing the **F8** key.

   (Do not press **F2** to go into *BIOS*, because there you can easily make your PC unable to boot.)

3. Wait until the boot device menu appears, select removable device with the **ARROW KEY DOWN** → **ENTER**

4. The '*Windows Setup*' screen appears:

   a) You see at the bottom of the window '*Setup is loading files*'.

   b) You see at the bottom of the window '*Setup is starting Windows XP*'.

5. A '*Windows XP Professional Setup - Welcome to Setup*' screen will appear with the Option of Continuing Setup, Repair a previous installation, or Quitting:

   a) Press **ENTER** to Continue Setup.

6. A text about the "Windows XP Licensing Agreement" (EULA) screen will appear:

   • Press the **PGDN** key repeatedly until the end, press **F8** (to accept).

   You see at the bottom of the window '*Searching for previous versions of Microsoft Windows*'.

7. If you have already other Windows XP installations on your PC, a list of them will appear. Press ESC in order to make a new installation instead of repairing an older one

8. If you have a couple of partitions on your hard disk, a list of currently available partitions will appear:

   a) Press the **ARROW UP** or **DOWN** key to highlight the partition on which Windows XP must be installed.

   b) Press **ENTER**

      • Select **Format the partition using the NTFS file system**, press **ENTER**

! You are asked if you really want to format this partition or want to choose a different partition. After this point formatting will be started, ALL DATA ON THIS PARTITION WILL BE LOST! Data on other partitions (which might be on the same disk) remain untouched. If you want to format this partition, press **F** (to start formatting) and wait...

9. A window '*Your Computer will reboot in 15 s*' will appear

   Remove any Floppy but keep the CD in its drive.

10. After the reboot the setup will continue automatically

    A window '*Windows XP Setup*' occurs, please wait ...

11. A window '*Windows XP Professional Setup*' will appear:

    a) Click **NEXT** or wait for a short time

    b) Installing Devices (wait ...)

    c) '*Regional Settings*'

       • Normally you could leave English (United States) for system locale. Set the right keyboard layout → **NEXT**

    d) '*Personalize Your Software*'

       • Type in your name and organization → **NEXT**

    e) '*Your Product Key*' (see on the top of the PC):

       • Enter the **Product ID** which is specified on the manual '*Microsoft Windows XP Professional*' (on the Certificate of Authenticity) → **NEXT**

    f) '*Computer Name and Administrator Password*':

       • Enter the **Name** (hostname) you have chosen for your computer

         Note that the first character must be alphanumeric and underscores are not allowed

       • Choose an Administrator password and enter it in the field **Password**, enter the same password in the field **Confirm Password**→ **NEXT**

! Important: remember the Administrator password.

    g) '*Date and Time Settings*'

       • Check if Date&Time are set correctly, change if necessary

         Select the correct time zone for your location, e.g.:

> GMT + 01:00 for Germany
> GMT - 05:00 for the US east coast
> GMT - 08:00 for the US west coast

- click **NEXT**

h) '*Networking Settings*' (wait ...)

- Enable Typical Settings→ **NEXT**

i) '*Workgroup or Computer Domain*'

- To get this information contact your system administrator, if you are not sure at the moment, please choose '*No, this computer is not on a network ...*' and enter the workgroup name → **NEXT**, please wait ...

j) The text '*Performing Final Tasks*' appears:

- please wait ...

k) The text '*Completing the Windows XP Setup Wizard*' appears:

- click **FINISH**, the system will reboot

l) Eject the CD-ROM

12. A window '*Network Identification*' will appear → **NEXT**

a) Users of this computer - who can log on to this computer?

- Enable '*Users must enter a user name ...*', click **NEXT** → **FINISH**

You can log in as Administrator using the password which you have entered during the installation.

11.2 Installing Windows XP Service Pack

PCs from Bruker Biospin are delivered with the latest Service Pack available at the time of delivery. Under Windows XP it is not necessary to reinstall the service pack after e. g. configuring the network.

The Service Pack can be downloaded from www.microsoft.com or www.microsoft.de.

For installation just follow the given instructions on the screen.

11.3 Installing the Graphics driver

Hewlett Packard PCs from Bruker BioSpin are delivered with the Graphics driver on the CD. If you do not have a floppy or a CD and want to install a newer driver, you can download a Graphics driver from the Web. Go to:

```
http://h20000.www2.hp.com/bizsupport/TechSupport/Product.jsp?prod-
TypeId=12454&prodCatId=296720&locale=en_US&taskId=135
```

The Graphics drivers are offered as self-extracting .exe files. Just download the file for your system, then click its icon and insert a formatted floppy. This way, you can create a new Graphics driver floppy.

The Graphics driver CD can be installed as follows:

1. Insert the Graphics driver CD
2. Click **Start** → **Control Panel**
3. A window '*Control Panel*' will appear:
   - Double-click the icon **Display**
4. A window '*Display Properties*' will appear:
   - Click **Settings**
5. If the window 'Invalid Display Settings' appears: click **OK**
6. Click **Advanced** → **Adapter** → **Properties** → **Driver** → **Update Driver**→ **Next** → enable **'Display a List ...'** → **Have Disk**
7. A window '*Install From Disk*' will appear:

   Enter your CDROM, e.g. **d:** or accept the default if it is correct → Click **OK**
8. The Graphics driver which resides on the CDROM will appear: Click **OK**
9. A window '*Third-party Drivers*' will appear:
   - Click **Yes** (to proceed) and wait ...
10. A window '*Installing Driver*' will appear: click **OK**
11. In the window '*Upgrade Device Driver Wizard*': click **Finish**
12. Close the windows you have just opened
13. Remove the CD
14. A window '*Systems Settings Change*' will appear: click **Yes** (to reboot)

The procedure for other PC's or other Graphics drivers might be a little different.

Chapter 12

Configuring Windows XP

12.1 Conversion of disk format from FAT to NTFS

Windows XP supports three file systems for disks: FAT16, FAT32, and NTFS.

Bruker BioSpin TOPSPIN and the datasets of the NMR experiments requires the file format NTFS. So if you use a FAT-partition of your harddisk(s), you have to convert this partition to 'NTFS' (that is the file system of Windows XP) before you can install the TOPSPIN. Only under NTFS, it is possible to have the file permissions, ownership and access management settings that make Windows XP secure. You can use the convert command `convert.exe` to convert an existing FAT volume to NTFS. Because this conversion retains all of your files, use `convert.exe` when you want to keep existing files on your volumes intact.

The conversion to NTFS is a one-way process. After you convert a drive or partition to NTFS, you cannot convert it back to FAT. To restore the volume to the previous file system, you must format it as FAT again. This action erases all existing data including your programs and personal files. In this case, you must either restore your data from a backup, or reinstall your operating system and programs.

`convert.exe` requires that you have a certain amount of free space on the drive or partition to convert it. If `convert.exe` determines that there is not enough free space on the volume, it does not convert the volume.

12.1.1 Check the Disk Partitioning

To check the configuration of the disk(s) of your PC, please start up the Disk Administrator utility from the command menus as shown below:

1. Click **Start** → **Control Panel** → **Administrative Tools**
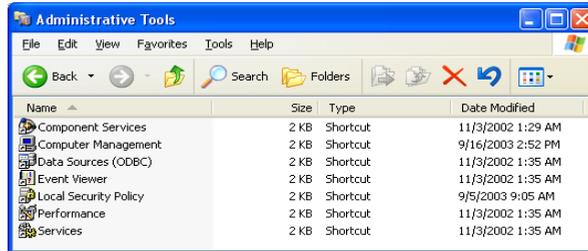
2. Click on **Computer Management** → **Disk Management**
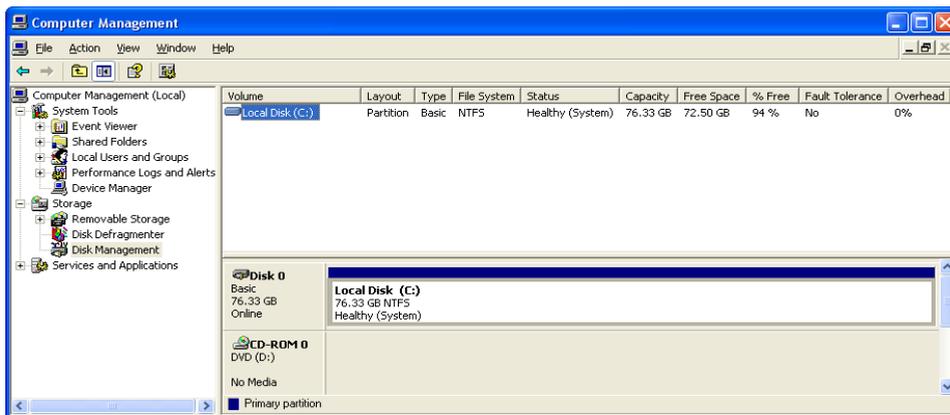
If this is the first time you start Disk Administrator, you probably see two information screens which you can confirm by clicking **OK,** respectively **Yes**:
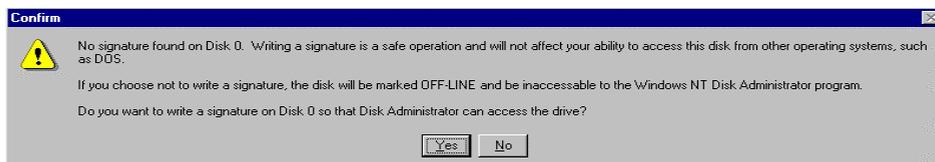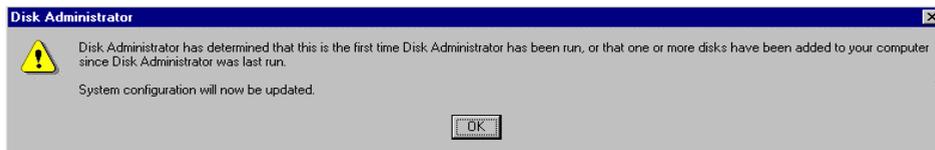
Finally, the disk administrator will show you how many disk drives your system has, and how they are partitioned.

Please realize that repartitioning the C: partition involves re-installing Windows XP!

Also, the maximum partition size with FAT is 4 GByte, with NTFS 7.8 GByte. Nevertheless, if you decide to make changes in the partitioning now is a good time to do it because you did not invest too much time in configuration and installation yet (e. g. the TOPSPIN is not installed and configured so far). All other partitions are usually empty at delivery of the PC and you can re-partition them or assign different drive letters. An other file system format is FAT32 that has the advanced of none maximum partition size and that could be read by windows 9x, NT and 2000.

12.1.2 Converting partitions from FAT to NTFS

You see that in our case, both C: and D: already have the NTFS file system. If, on your system, partition D: or any other partition on which you want to store NMR data is FAT, you can change that from the Disk Administrator. Just click

All Tasks → **Format** from the **Action** menu, select the NTFS file system and Start formatting.

Be aware that this will erase the entire partition.

The C: drive cannot be converted from the disk administrator. It can, however, be scheduled for conversion during the next boot up. In this way, the entire contents of C:, like Windows XP, will remain intact. Important: This is again a critical operation concerning power loss. If the conversion runs and the power goes away it will render the disk unusable and Windows XP must be re-installed. So it might be a good idea your PC to connect to an Uninterrupted Power Supply before you move on.

To convert a drive from FAT to NTFS without loss of data, start a Command Prompt from the command menus: Then type the following command on the command line and press return:

```
convert  <drive:>  /fs:ntfs
```

The system will ask you to schedule the actual conversion for the next boot-up and

you will reply with '**y**' as shown below:
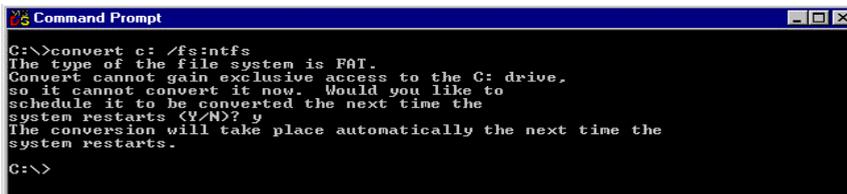
you do NOT need to re-boot now and wait the 2-3 minutes for it to complete. Just move on with the operations explained in the next chapter. The conversion to NTFS will automatically be done during the next re-boot.

12.1.3 Cutting down the re-boot time

1. Click **Start** → **Control Panel** → double click on **System**

A window '*System Properties*' will appear:

2. Click **Advanced** → **Startup and Recovery**:
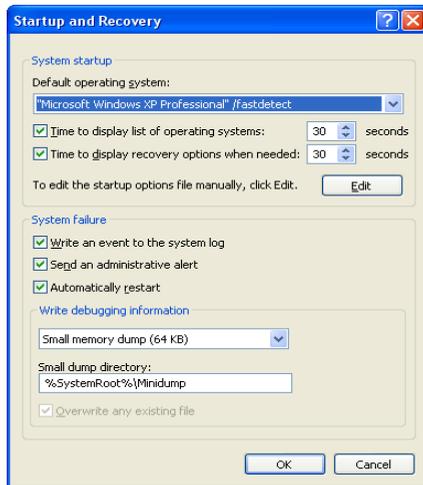
The default entry for the time the system waits for your boot selection during boot up is set to 30 seconds. You can set this entry to 5 seconds which is usually enough to select a different boot mode (or partition) if you want to do that.

3. Click **OK**

Chapter 13

Windows XP Networking

!

In order to run TOPSPIN, you must setup the network (TCP/IP protocol), even if your PC is not connected to a spectrometer or to the laboratory network.[1] You can setup the network as a so-called Domain scenario or as Workgroup scenario. This chapter describes the Workgroup scenario.

13.1 TCP/IP configuration

This chapter describes how to install both the laboratory network (Workgroup scenario) and the spectrometer internal network for a 'hp workstation xw4400'. The description for other PC's with a different Ethernet card might be a little different. Before you start, make sure all network hardware components (network card, adapter, cables etc.) are properly connected. Then make a list of the following information:

- IP address for the PC in the laboratory network
- subnet mask of the laboratory network
- DNS domainname of the laboratory network
- IP address of the DNS nameserver(s) (if a nameserver exists)

---

1. The TOPSPIN license requires TCP/IP to be installed.

- IP address of the default gateway (if a default gateway exists)

If your PC is not physically connected to the laboratory network, you can use any IP address, subnet mask and domainname for the (external) network configuration. A frequently used IP address for such a 'standalone' computer is 192.168.0.1. This address is not assigned to any network computer (by world-wide-agreement). However, for the spectrometer internal network, you must use the values as specified below.

Perform the following steps according to the necessities of your setup:

13.1.1 Create a New Network Connection

1. Log in as Administrator
2. Click **Start → Control Panel → Network Connections**
3. A window *Network Connections* will appear
4. Click on **Create a new connection** on the left side of the window
5. A window *Network Connection Wizard* will appear → **NEXT**
6. Enable **Connect to the Internet → NEXT**
7. A window *Now Getting Ready* will appear
8. Enable **Connect using a broadband connection that is always on → NEXT**
9. A window *Completing the New Connection Wizard* will appear → Click **FINISH**

13.1.2 Configuring the TCP/IP of an existing Network Connection

1. Log in as Administrator
2. Click **Start → Control Panel → Network Connections**
3. A window '*Network Connections*' will appear
4. Highlight the connection you want to configure → **File → Properties**
5. Highlight the TCP/IP entry and click **Properties**
6. The window '*Internet Protocol (TCP/IP) Properties*' will appear:
7. Enable '*Use the following IP address*'
   b) In the field **IP Address**: enter the IP address of your computer
   c) In the field **Subnet Mask**: enter the subnet mask of your network

e.g. 255.255.255.0 or 255.255.0.0

d) In the field **Default Gateway**: enter the IP address of the Default Gateway in your network (if available)

e) If you have a nameserver:

- In the field **Prefered DNS Server** enter the IP address of the nameserver
- If you have a second nameserver enter his IP address in the field '*Alternate DNS server*'

f) Click **Advanced → DNS**

g) Enable the field **Append these DNS suffixes (in order) → Add**

- In the window '*TCP/IP Domain Suffix*':

  Enter the network domainname → **Add**

h) Click **OK**

i) If the question appears:

'This connection has an empty primary WINS address. Do you want to continue?' → **YES → OK → OK → CLOSE**

13.1.3 Configuring the TCP/IP with DHCP of an existing Network Connection

This chapter describes how to configure the TCP/IP of an existing Network Connection for DHCP (Dynamic Host Configuration Protocol)

1. Log in as Administrator

2. Click **Start → Control Panel → Network Connections**

3. A window '*Network Connections*' will appear

4. Highlight the connection you want to configure → **File → Properties**

5. Highlight the TCP/IP entry and click **Properties**

6. The window '*Internet Protocol (TCP/IP) Properties*' will appear. Select the options:

- Enable **IP address automatically**

- Enable **DNS server address automatically**
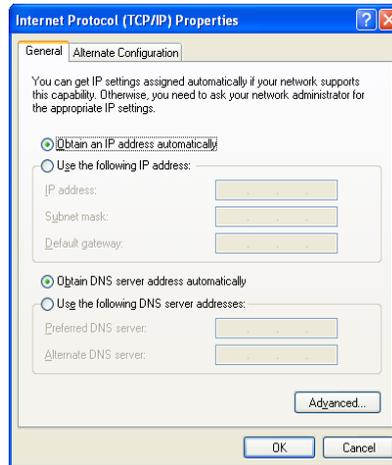
7. Click on *Advanced*. A window '*Advanced TCP/IP Settings*' will appear:
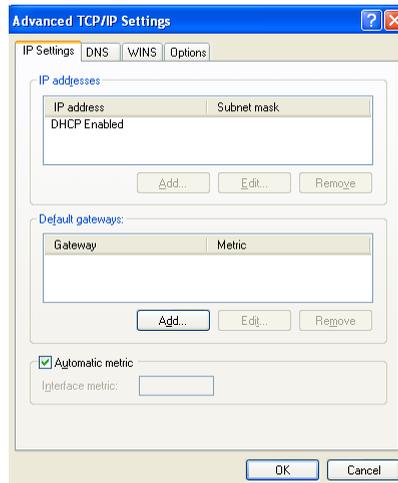
8. Ensure that the *Default gateways* box is empty. If not: select each entry and click on the **Remove** button.

9. Select the *DNS* tab.
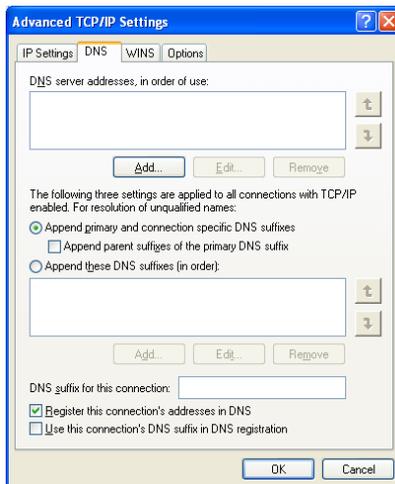
10. Select the **Register this connection's addresses in DNS** option.

11. Check that the **DNS server addresses**, **in order of use** and **Append these DNS suffixes (in order)** boxes are empty. If not: select each entry and click the **Remove** button.

12. Select the **WINS** tab.

13. The **WINS addresses**, **in order of use** should be empty. If not: select each entry and click the **Remove** button.

14. Click → **OK** → **OK** → **CLOSE**

15. If you are asked to restart your computer: Click **Yes**.

16. After your computer has been restarted, Windows will automatically request network information from the DHCP server.

13.1.4 Configuring the TCP/IP of the Spectrometer Control:

1. Log in as Administrator

2. Click **Start** → **Control Panel** → **Network Connections**

3. A window '*Network Connections*' will appear

4. Highlight the connection you want to configure → **File** → **Properties**

5. Highlight the TCP/IP entry and click **Properties**

6. The window '*Internet Protocol (TCP/IP) Properties*' will appear:

   • In the field **IP Address**: enter **149.236.99.1**

   • In the field **Subnet Mask**: enter **255.255.255.0**

   For the spectrometer network ONLY THESE VALUES ARE VALID!

   Do not choose different settings for the IP address or Subnet mask.

   • Leave the Field Default Gateway empty

7. Click **OK**

If your PC controls a spectrometer we recommend to do the following:

1. Click **Start** → **Control Panel** → **Network Connections**

2. A window '*Network Connections*' will appear:

   a) Select the Adaptor to which the spectrometer CCU is connected. This is nor-
      mally, but not necessarily Adaptor 2.

   b) Right mouse click → **Properties**

   c) Disable the entry **Client for Microsoft Network (TCP/IP) by** clicking on
      the '**+**' sign to the left of the entry

13.2 Changing the hostname of the computer and its effects

If you want to change the hostname of your PC you can do this in the following
way. IMPORTANT: You also have to change the text-file:

`<TOPSPINHOME>\conf\nmrsuperuser`

This file contains the computer-name and the Windows XP user which is the TOP-
SPIN-SUPERUSER. You can edit and change this file with a normal text editor like
notepad if you are logged in as the Windows XP-user which is the NMRSUPE-
RUSER.

1. Log in as Administrator

2. Click **Start** → **Control Panel** → **Network Connections**

3. A window '*Network Connections*' will appear:

   a) Click **Advanced** → **Network Identification**

   b) A window '*System Properties*' will appear

   c) Click **Network Identification** → **Properties**

  d) In the field **Computer Name**: enter the new hostname

Note that the first character must be alphanumeric and underscores are not allowed!

  e) Click **OK**

4. A window '*Network Identification*' will appear:

- Click **OK**

5. In the window '*System Properties*':

- Click **Close**

6. A window '*System Setting Change*' will appear:

- Answer the question if you want to restart the computer now by clicking **Yes**

7. If you have *Floating* licenses you must change the hostname in the file license.dat. By default it resides in C:\flexlm\Bruker\licenses. You can do this in the following way:

  a) Click **Start → All Programs → Accessories → Command Prompt**

  b) Enter: **cd c:\flexlm\Bruker\licenses**

  c) Enter: **notepad license.dat**

   - Change the hostname in the SERVER line, then save and exit the file.

Of course, you can also change the license file from the Explorer. We have chosen the Command Prompt because the Explorer might add the (hidden) extension .txt to the file license.dat which makes it unusable (see chapter 16.1.3).

13.3 Network diagnostic commands

Here is a list of the most important network diagnostic commands as they can be entered from the Command Prompt:

- **arp** - displays or modifies the IP to physical address translation tables
- **hostname** - displays the name of the current host
- **ipconfig** - displays information about the current TCP/IP configuration
- **netstat** - displays protocol statistics and current TCP/IP connections
- **ping** - checks if a destination host is receiving TCP/IP packets

- **`route`** - maintains and displays routing tables
- **`tracert`** - displays the route packets take to a destination host
- **`net start`** - displays all running services
- **`net use`** - display current network connection
- **`nbtstat -a`** - displays all registered NetBIOS names

13.4 Accessing remote files and directories

13.4.1 Sharing directories from a Windows XP host

Network operations under Windows XP primarily takes place via the Windows XP sharing mechanism. For example, you can share the data directory `c:\data` on *nthost_a* by taking the following steps:

1. Log in as Administrator on *nthost_a*

2. Open drive `C:` in the Explorer

3. Right-click on **data**

4. A popup window will appear:

   Click **Sharing and Security**

5. A window '*Data Properties*' will appear:

   a) Click **Share this folder**

   - Accept the default shared name *data*, or enter any other name [1]
   - Optionally, you can enter a comment

   b) Optionally, you can set a user limit and/or shared permissions
   (note that the default permissions are Full Control for Everyone)

   c) Click **OK**

The directory `c:\data` can now be accessed from any Windows XP host in the network, e.g. from *nthost_b*, in the following way:

1. Log in on *nthost_b* as normal user

2. Click the icon **My Network Places** on the desktop

---

1. This is the name under which the directory can be accessed from other hosts

3. A list of hosts in the network will appear:

- Double-click the icon of *nthost_a*

4. A window '*Enter Network Password*' will appear:

a) In the field **Connect As**: enter the name of any user on *nthost_a*

b) In the field **Password**: enter the password for this user

   → A list of shared partitions/directories will appear

   (The network password is only requested for the first connection).

Now you can:

- Access the remote directory as if it were local
- Copy the remote directory or any sub-directory or file in it, by dragging the corresponding icon into any target directory window (assuming you have the write permission in the target directory).

Note that the latter is only useful if the remote directory is not permanently shared.

13.4.2 Enabling and disabling Simple File Sharing

A PC under Windows XP Professional that is joined to a <u>workgroup</u> has the Simple File Sharing enabled by default. The Simple File Sharing is located in the folder's properties. When you set the Simple File Sharing the share and the file permissions are configured.

A Windows XP Professional PC that is joined to a <u>domain</u> use only the classic file sharing and security interface.

If you disable Simple File Sharing, the Shared Documents feature is not turned off.

You have more control over the permissions to individual users, if you disable the Simple File Sharing, However, you must have advanced knowledge of NTFS and share permissions to keep your folders and files secure.

It is recommended that you share folders only on the network within your user profile that remote users on other computers need to access. Never ever share the root of your system drive. In this case your computer is more vulnerable to malicious remote users.

To turn Simple File Sharing on or off:

1. Double-click **My Computer** on the desktop.

2. Click on **Tools**, select **Folder Options**.

3. Click the **View** tab, then click to clear the **Use Simple File Sharing (recommended)** check box to disable Simple File Sharing.

4. Click **OK**.

Levels of Access

There are five levels of access:

1. Level 1: My Documents (Private)

2. Level 2: My Documents (Default)

3. Level 3: Files in shared documents available to local users

4. Level 4: Shared Files on the Network (Readable by Everyone)

5. Level 5: Shared Files on the Network (Readable and Writable by Everyone)

In Levels 1, 2, and 3 folders are available only to a user who is logging on locally. Levels 4 and 5 folders are available to users who log on locally and remote users from the network .

You can have the following permissions:

Access Level	Everyone (NTFS/File)	Owner	System	Administrators	Everyone (Share)
Level 1	no	Full Control	Full Control	no	no
Level 2	no	Full Control	Full Control	Full Control	no
Level 3	Read	Full Control	Full Control	Full Control	no
Level 4	Read	Full Control	Full Control	Full Control	Read
Level 5	Change	Full Control	Full Control	Full Control	Full Control

1. Level 1: My Documents (Private)

   Only the owner of the file or folder has the permission to read and write to the file or folder. All subfolders that are contained within a folder that is marked as private remain private unless you change the parent folder permissions. The option to make a folder private is only available to a user account in its own *My Documents* folder.

   To Configure a folder and all of the files in it to Level 1:

   a) Right-click the folder → click **Sharing and Security**.

   b) Click to select the **Make this Folder Private** check box → click **OK**.

2. Level 2 (Default): My Documents (Default)

   Only the owner of the file/folder and a local administrator have the permission to read and write to the file/folder. This is the default setting for all of the folders and files in each user's *My Documents* folder.

   To configure a folder and all of the files in it to Level 2:

   a) Right-click the folder → click **Sharing and Security**.

   b) Ensure that both the **Make this Folder Private** and the **Share this folder on the network** check boxes are cleared → click **OK**.

3. Level 3: Files in Shared Documents Available to Local Users

   Files are shared with users who log on to the computer locally. Local administrators and Power Users can read, write, and delete the files in the Shared Documents folder. Restricted Users can only read the files in this folder. In order to allow Remote Users to access folders/files at Level 3, you must share them out on the network (Level 4 or 5).

   To configure a file/folder and all of the files in it to Level 3:

   a) Start Microsoft Windows Explorer

   b) Copy or move the file/folder to the Shared Documents folder under My Computer.

4. Level 4: Shared on the Network (Read Only)

   For everyone on the network and local users (including the Guest account (if activated)) the files are shared to read. But they are not allowed to modify the contents. User that can connect to the computer on the network are able to read and change these files.

   To configure a folder and all of the files in it to Level 4:

    a) Right-click the folder $\rightarrow$ click **Sharing and Security**.

    b) Click to select the **Share this folder on the network** check box

    c) Click to clear the **Allow network users to change my files** check box $\rightarrow$ click **OK**.

5. Level 5: Shared on the Network (Read and Write)

This level is recommended only for a closed protected network that has a firewall configured.

This level is the most available and least secure of all access levels. Any user can read, write, change, or delete a file in a folder shared at this access level.

To configure a folder and all of the files in it to Level 5:

    a) Right-click the folder $\rightarrow$ click **Sharing and Security**

    b) Click to select the **Share this folder on the network** check box $\rightarrow$ click **OK**.

NOTE: All NTFS permissions that refer to Everyone include the Guest account.

13.4.3 Sharing directories from a UNIX host using Samba

If you are logged in on a Windows XP host, you can access data which reside on a UNIX host, using the sharing mechanism. This, however, only works if the Samba package is installed on the UNIX host. For further information please see the TOP-SPIN Installation Guide for Linux. You can download this Installation Guide as the up to date version from the Bruker web-server:

```
http://www.bruker-biospin.de/NMR/nmr-
     softw/passwd/docu/index.html
```

13.4.4 Mounting Windows XP partitions from a UNIX host using NFS

If your PC is controlling a spectrometer, installation of the Hummingbird NFS Server is mandatory. The partition `C:\Bruker\Diskless\clients\spect` is mounted via NFS by the spectrometer CCU (which is a UNIX host). In the same way, you can mount any Windows XP partition or directory on any UNIX host. Proceed as follows:

1. Export the Windows XP partition as described in chapter 6.6.1. In step 4, you must enter the partition and, optionally, the UNIX host(s) to which it must be exported.

2. On the UNIX host:

   a) Open a UNIX shell

   b) Type **su** to become superuser

   c) Create a mount directory, e.g. **mkdir /ntdata**

   d) mount the partition, e.g.:

   - on SGI: **mount nthost:/c/data /ntdata**

   - on X32: **mount -f NFS nthost:/c/data /ntdata**

   Note that, if the pathname on the Windows XP hosts contains uppercase letters, these must also be specified with the mount command.

13.4.5 FTP

Network transfer under Windows XP is generally done via the directory sharing as described in chapter 13.4.1 and 13.4.3. Nevertheless, Windows XP supports transfer via FTP. Just enter '**ftp hostname**' from a Command Prompt and you can transfer files.

13.4.6 Telnet

Windows XP contains a **telnet** command for remote login. Just enter **telnet hostname** in a Command Prompt to login to a remote host. The telnet command can only be used to login from your PC to a remote host (e.g. a UNIX host) but not vice versa.

With Windows XP it is also possible to do a telnet login to a Windows XP computer but this feature is not very convenient.

13.5 Outlook Express

Alternatively to printing and faxing diagnostics results to Bruker BioSpin or somewhere else, you can send the same information via electronic mail. For this to work, the spectrometer PC needs access to the Internet, i.e. to an Internet gateway in your local network.

Install a program that allows for composing and sending e-mail messages. If you have **Microsoft Internet Explorer 6.0** or newer, we recommend to install it. Internet Explorer is bundled with an e-mail application called **Outlook Express**.

13.5.1 Installation and configuration of Outlook Express

Outlook Express gets automatically installed with Microsoft Internet Explorer 6.0 or newer.

- Open **Start** → **All Programs** →**Outlook Express**
- or double-click the **Outlook Express** icon on the desktop.

Supply all parameters asked for by the setup wizard. Contact your network administrator if you are not sure what to fill in.

Select **Options** from Outlook Express' **Tools** menu and configure the General Settings as shown below.
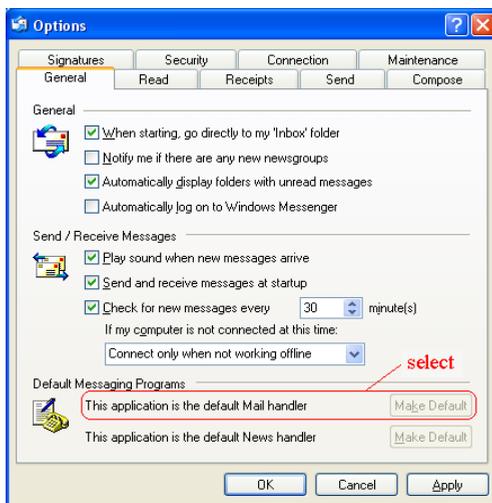
Outlook Express version 6 is able to handle the default mail handling and the simple MAPI client as one. It is sufficient to enable the setting as default mail program

Do not reboot the computer now. Open the **Options** interface again, switch to the

Send page and select the topics as shown below.
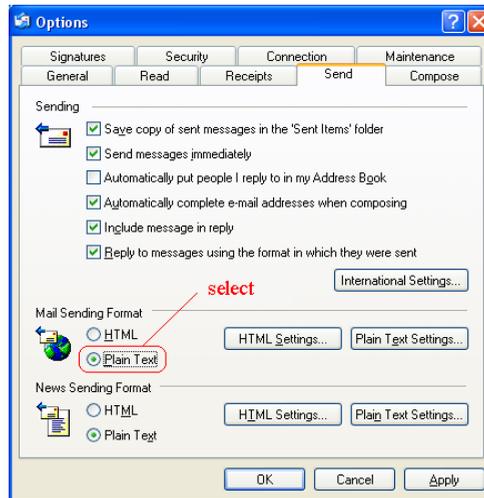
Switch to the **Security** page and disable *Warn me when other applications try to send mail as me*, then reboot the computer.
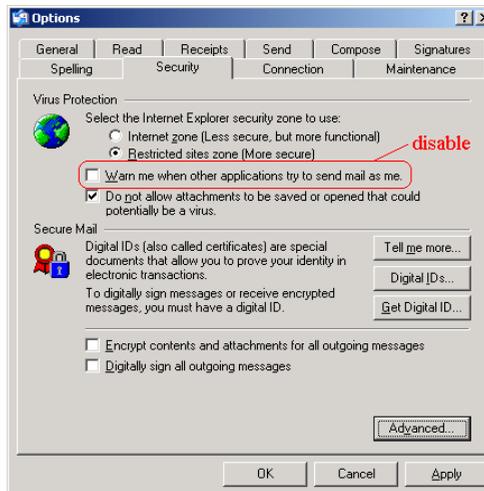
To disable this warning might be a security leck. If you do not disable this warning, you get a warning every time if ICON-NMR send an e-mail.

13.5.2 Sending an e-mail with Outlook Express

- Fill in the correct recipient's address.

- Click the **Send** button.

If you want to use an e-mail application not mentioned here, make sure it has some 'use as simple MAPI client' feature and activate it.

13.6 Installing the TOPSPIN in a Windows XP Domain

Windows XP provides two different security scenarios for computer networks, the Workgroup and the Domain scenario. With a Workgroup scenario, each computer has its own local security database of user accounts and passwords. This means that users from workstation A are not known at workstation B. They might have the same name on both workstations but internally they are represented by two different security identifiers. Users from workstation A can access files on workstation B via the sharing mechanism (see chapter 13.4.1). The Workgroup scenario is typically used for small networks. For large networks, the Domain scenario is usually preferred. In this case, one computer (the Domain Controller, DC) maintains the security database for an entire group of Windows XP Computers. A Domain user can log on at each workstation in the Domain with a single account and password. Furthermore, the Domain Administrator's account has administration rights on every computer in the Domain. Nevertheless, a local Administrator account exists on each computer for local administration tasks.

Bruker BioSpin TOPSPIN fully supports both security scenarios. The description of the TOPSPIN installation in chapter 6.4 is valid for a Workgroup scenario. This chapter describes the additional installation steps which are required for a Domain scenario. The NMR Superuser (see chapter 6.2), which is specified during the installation of TOPSPIN can now be a local account or a Domain account. In both cases the NMR Superuser only needs standard access permissions. The installation of TOPSPIN, however, requires Administrator rights because certain system services and two user groups are installed. Furthermore:
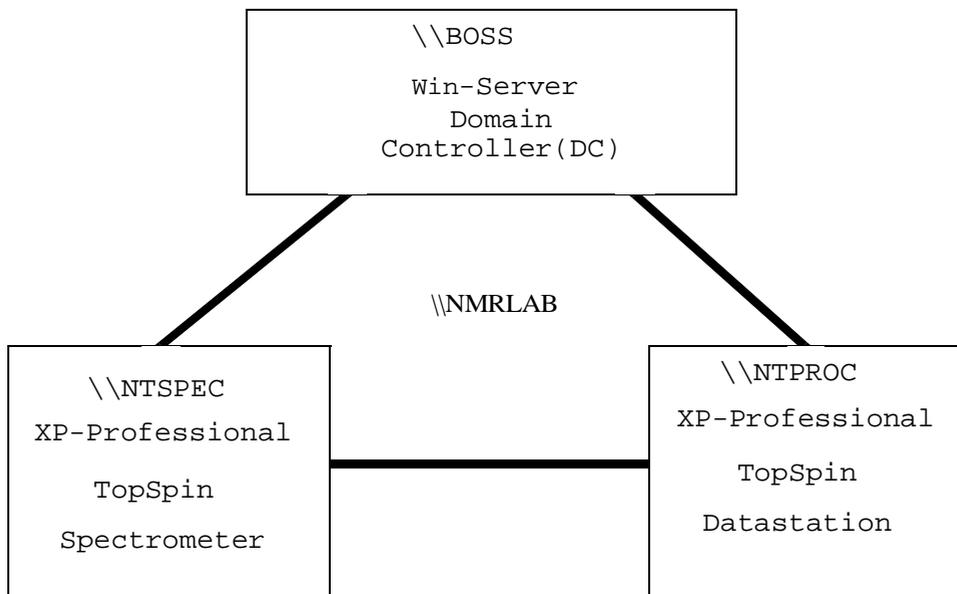
<div align="center">

TOPSPIN must be installed as <u>local</u> Administrator

</div>

This means no Domain-wide administrative tasks are done during the installation. The installation of TOPSPIN in a Domain involves the following steps:

1. Make sure that there is a Local or Domain account for NMR Superuser, or create one.

2. Installation of TOPSPIN by the local Administrator.

3. Creation and configuration of global groups of NMR users by the Domain Administrator.

4. Make sure that all nmr users have an existing HOME directory

As an example, we use a Domain *NMRLAB* with two workstations; *NTSPEC* which controls a spectrometer and *NTPROC* which is used for processing. The security database resides on the Domain Controller *BOSS*. Step 2, the installation of TOPSPIN is the same on *NTSPECT* and *NTPROC* so it will only be described for *NTSPEC*.

```
            ┌─────────────────────────┐
            │        \\BOSS           │
            │                         │
            │       Win-Server        │
            │         Domain          │
            │     Controller(DC)      │
            └─────────────────────────┘

                    \\NMRLAB

┌─────────────────────────┐         ┌─────────────────────────┐
│       \\NTSPEC          │         │       \\NTPROC          │
│    XP-Professional      │         │    XP-Professional      │
│                         │         │                         │
│       TopSpin           │         │       TopSpin           │
│                         │         │                         │
│     Spectrometer        │         │     Datastation         │
└─────────────────────────┘         └─────────────────────────┘
```

13.6.1 Creating an NMR Superuser account

Before you install TOPSPIN, you have to make sure that there is an account for NMR Superuser. If there is none which you like to use, create a new one. According to your preference this can either be a local or a Domain account.

a) Creating a <u>local</u> NMR Superuser account

If you prefer a local NMR Superuser, do the following:

1. Log on at Windows XP Professional Workstation *NTSPEC* as the local Administrator or any other user who has User Administration rights, selecting *NTSPEC* as Domain.

2. Open the User Manager and create an account for the NMR Superuser, e.g. with the name *nmrsu*. (see also chapter and 9.1).

b) Creating a <u>Domain</u> NMR Superuser account

If you prefer a Domain NMR Superuser, do the following:

1. Log on at the Domain Controller *BOSS* as the <u>Domain</u> Administrator.

2. Open the User Manager and create an account for the NMR Superuser, e.g. with the name *nmrsu* (see also chapter and 9.1).

Note that the installation of TOPSPIN, which must be done as local Administrator, relies on the fact that the NMR Superuser was correctly installed. It cannot check if a Domain NMR Superuser really exists.

c) Installing TOPSPIN

The installation of TOPSPIN involves the following steps:

1. Log on as <u>local</u> Administrator on Windows XP Professional *NTSPEC*.

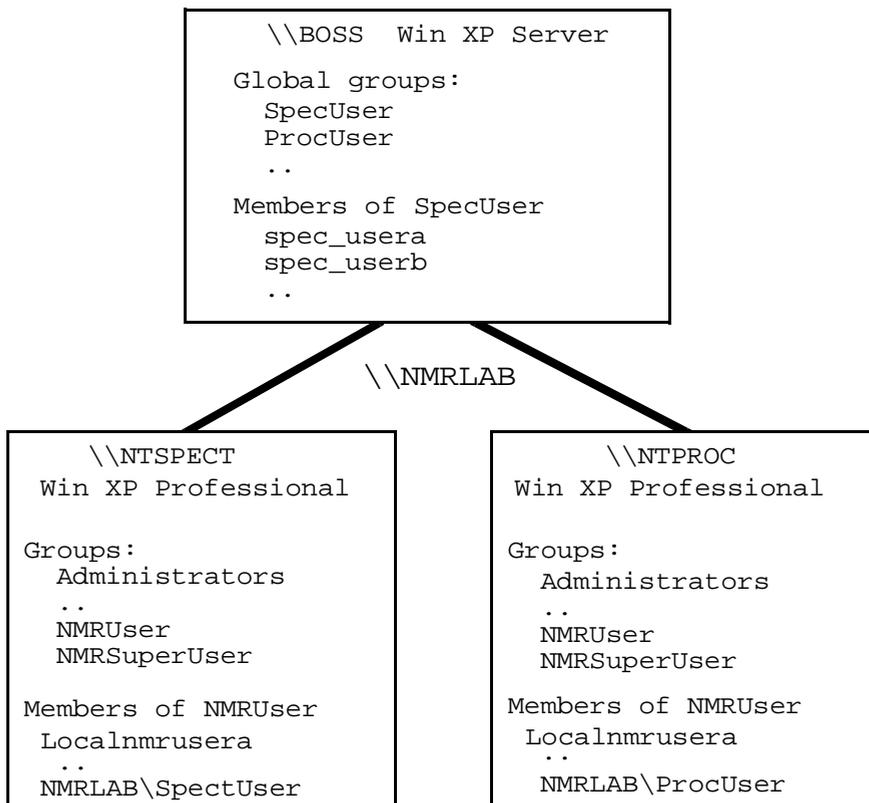**2.** Install the TOPSPIN as described in chapter 6.4.

During the installation process, you will be asked for the NMR Superuser. Enter the name of the NMR Superuser account as created before (see chapter 13.6.1).

After the installation process, NMR users cannot start TOPSPIN yet. First they must be added to the local group NmrUser. Users with a <u>local</u> account, e.g. localnmrusera can simply be added to NmrUser as described in chapter 9.1.3. However, for users with a <u>Domain</u> account, which is typical in a Domain scenario, we recommend to use global groups as described in chapter 13.6.2.

13.6.2 Installing global user groups

The TOPSPIN installation program creates a local group NmrUser. Each user who wants to use TOPSPIN must be a member of this group. Domain users could be added individually to the local group NmrUser but, in a network with many Workstations and varying users, this would be an elaborate task. Therefore, we recommend to create so called <u>global</u> user groups. Global groups are created by the Domain Administrator on the Domain Controller. Each global group contains users who are allowed to do certain tasks, e.g. start TOPSPIN on a specific spectrometer or datastation. These global groups are then added to the local group NmrUser on the various Workstations in the network. In our example, the Domain Administrator creates the global groups *SpecUser*s and *ProcUsers* which are then added to the local group NmrUser on *NTSPEC* and *NTPROC* respectively. After

that, for example, the global user spec_usera can control the spectrometer from Workstation *NTSPEC*. By managing these global groups on the Domain Controller, the Domain Administrator can control which users can use the spectrometer and which can use the datastation. In practice, one global group will be added to the local group NmrUser on several Workstations and NmrUser on one Workstation can contain several global groups.

```
┌─────────────────────────────────────────┐
│        \\BOSS  Win XP Server            │
│                                          │
│    Global groups:                        │
│      SpecUser                            │
│      ProcUser                            │
│      ..                                  │
│                                          │
│    Members of SpecUser                   │
│      spec_usera                          │
│      spec_userb                          │
│      ..                                  │
└─────────────────────────────────────────┘

                  \\NMRLAB

┌──────────────────────────┐   ┌──────────────────────────┐
│      \\NTSPECT           │   │        \\NTPROC          │
│   Win XP Professional    │   │   Win XP Professional    │
│                          │   │                          │
│  Groups:                 │   │  Groups:                 │
│    Administrators        │   │    Administrators        │
│    ..                    │   │    ..                    │
│    NMRUser               │   │    NMRUser               │
│    NMRSuperUser          │   │    NMRSuperUser          │
│                          │   │                          │
│  Members of NMRUser      │   │  Members of NMRUser      │
│   Localnmrusera          │   │   Localnmrusera          │
│    ..                    │   │    ..                    │
│   NMRLAB\SpectUser       │   │    NMRLAB\ProcUser       │
└──────────────────────────┘   └──────────────────────────┘
```

The installation of the global user groups involves the following steps:

1. Log on at the Domain Controller as Domain Administrator.

2. Create the global groups *SpecUser* and *ProcUser*.

3. Log on as local Administrator at workstation *NTSPEC*, selecting *NTSPEC* as Domain.

4. Add the <u>global group</u> *NMRLAB\SpecUser* to the <u>local group</u> *NmrUser* as

described in chapter 9.2.4.

5. Repeat step 3 and 4 for *NTPROC* adding *NMRLAB\ProcUser* to the local group *NmrUser*.

13.6.3 Check for the HOME directory of every nmr users

There are two possibilities for the HOME directory of an user, local on every PC or fixed on one PC in the domain. Bruker supports both scenarios, the last one is a little bit more convenient, because the resource file (used by command 'setres') of TOPSPIN is stored in the home directory of the user. If there are individual settings it is easier to have to create this file only once and use it on all TOPSPIN installations of the windows domain.

Note that the configuration of TOPSPIN relies on the fact that the given HOME directory of an user exists. The HOME directory cannot be created by TOPSPIN.

Chapter 14

Installing a Printer

Printers must be installed at a Windows XP level and can then be used in TOPSPIN and TOPSPIN PLOT EDITOR.

14.1 Installing a new local printer

Installing a local printer implies installing the software, e.g. the printer driver for that printer. You can get printer drivers from various sources:

1. From a CDROM or floppy which was delivered with the printer:
   Please follow the instruction in the printer installation guide. If you do not have one, just insert the floppy or CDROM. The *Setup* program might start automatically. If it does not, open the Explorer and find a file named `Setup` or `Install` and click it.

2. From the Web:
   Just go to the manufacturers Web home page, e.g. `www.hp.com`, `www.canon.com` or `www.epson.com` and look for **Download** or **Drivers**. Usually, an executable file can be downloaded which can be unpacked and installed, simply by clicking on it.

3. From the Windows XP CDROM:
   If you do not have a CDROM or floppy with printer software and no Web access you can install a printer driver from your Windows XP CD. You will get

a list of printers for which a driver was available at the time your Windows XP version was released. If your printer type does not appear, you can select a related printer. However, Bruker BioSpin does not guarantee that this will work (see chapter 14.1.1 for installation instructions). Note:

Bruker BioSpin does not supply printer drivers for Windows XP!

14.1.1 Installing a printer from the Windows XP CDROM

A large number of printer drivers are available on the Windows XP CDROM. Note that these are the drivers which were available at the time Windows XP was released. For older printers these are usually valid. For newer printers the drivers might not be on the CD or better drivers might be available. Please use drivers delivered with the printer or from the Web whenever possible.

You can install a printer from the Windows XP CD as follows:

1. Log in as Administrator

2. Click **Start → Printers and Faxes**

3. A window '*Printers*' will appear:
   - Double-click the icon **Add Printer**

4. A window '*Add Printer Wizard*' will appear: → Click **NEXT**
   a) Click **Local Printer**, enable **Plug and Play** search mode if you want that the system looks for a new printer → Click **Next**
   b) A window '*New Printer Detection*' will appear
      - if the system finds a right printer → Click **Next**
      - if the system does not find a printer define it manually during the next steps → Click **Next**
   c) Select the port to which the printer is connected → Click **Next**
   d) In the field **Manufacturers**: select the manufacturer of the printer, e.g. HP
   e) In the field **Printers**: select the type of the printer

      If your printer does not appear in the list, select a related printer type or click **Cancel** and get the driver from the Web.
   f) Click **Next**
   g) In the field **Printer Name**: enter the name under which you want to use the printer (or accept the default name)

    h) If other printers are already installed, you will be asked if the new printer must be the default printer:

- If you want to use this printer as default printer → Click **Yes**

- If you do not want to use this printer as default printer → Click **No**

    i) Click **Next**

    j) '*Printer Sharing*': Do one of the following:

    If the printer must be available for other computers in the network:

- Click **Shared**
- In the field **Share Name**: enter the name by which the printer can be accessed from a remote host, e.g. *viola_deskjet*
- Click **Next**
- A window '*Location and Comment*' appears. Write in some informations about the location, the printer administrator and individual printer specifications (e. g. the fax-default-printer etc.) → Click **Next.**

    If this printer should only be used on the local computer:

- click **Not shared**.

    k) Click **Yes** (to print a test page) → Click **Next** → Click **Finish**

5. If the window '*Insert disk*' appears:

- Insert the CDROM '*Windows XP Professional*' → Click **OK**

6. A window '*Files Needed*' will appear:

- Click **OK** (to copy the Driver files for your printer from the CD)

7. A new icon will appear in the window '*Printers*' (see step 3):

    a) Click the right mouse button on the new printer's icon

    b) Click **Printing Preferences** in the pop-up menu

8. A window '*Printing Preferences*' will appear:

    a) Click **Advanced**

    a) Click in the Field **Paper Size**

    b) Select the correct paper size for your printer

    c) Click **OK** → **OK**

Step 8 makes sure that applications like Word, Excel, Paint and TOPSPIN ... will use this paper size as default.

14.2 Remote printing from a PC to a PC

14.2.1 On the PC to which the printer is physically connected

If the printer is not installed yet:

- Install the printer as described in chapter 14.1. During this installation you have to choose between 'shared' and 'not shared'; click **Shared**

If the printer is already installed as a local printer:

a) Log in as Administrator

b) Click **Start → Printers and Faxes**

c) Click the <u>right</u> mouse button on the printer icon and select **Sharing ...**

d) A window '*<printer name> properties*' will appear:

- Click **Shared**
- In the field **Share Name**: enter the name under which the printer can be accessed on the network, e.g. *viola_deskjet*
- Click **OK**

e) Close the window '*Printers*' by clicking the **X** button

14.2.2 On the PC from which you want to print

1. Click **Start → Printers and Faxes**

2. A window '*Printers*' will appear:

- Double-click the icon **Add Printer**

3. A window '*Add Printer Wizard*' will appear:

a) Click **Network printer**

b) Click **Next**

c) A window '*Locate your printer*' will appear, enable one of the three fields under the point '*What Do You Want To Do*'

- '*Find a Printer in the Directory*' is a powerful search tool that is looking for a printer with the properties you want in the active directory if you are member of domain

  - Click **Next**, a window '*Find Printers*' will appear:

- Choose the domain path in the field '*In*'

- In the menu '*Features*' you have the possibility to enable some additional search modes like resolution, paper size etc.

- Click **Find Now**

- '*Type the Printer Name ...*'

  - Use this option if you already knows whats the name of the printer you want to install (use the form //<Print-Server>/<Printer-Name>) or if you want to start a search in the subdomain of your network

  - Click **Next**

- '*Connect to a Printer ...*'

  - Use this option if you want to connect to a internet printer that has an own URL address

! Wait until list of shared printers on that UNIX host appears. If this list does not appear within one minute, click the **Network Connections** icon on the desktop and try to connect to the remote host. Then go back to the window '*Connect to printer*', click the remote host again and see if get a list of shared printers now.

4. The window '*Add Printer Wizard*' will appear:

  a) Do one of the following:

  - Click **Yes** if you want to use this printer as default printer

  - Click **No** if you do not want to use this printer as default printer

  b) Click **Next**, click **Finish**

14.3 Remote printing from a UNIX host to a PC

14.3.1 On the PC to which the printer is physically connected

Install the printer as described in chapter 14.2.1.

1. Log in as Administrator

2. Insert the CDROM '*Windows XP Professional*'

3. Close the window '*Windows XP CDROM*' by clicking **Exit**

4. Click **Start** → **Control Panel** → **Network Connection**

5. A window '*Network and Dial-up Connection*' will appear:

- Click on the pull down menu **Advanced → Optional Network Component**

6. A window '*Optional Network Component*' will appear:

- Enable **Other Network File and Print Services**

- Click on **Networking Services** to highlight it then click **Details**

  - enable **Simple TCP/IP Services → OK**

- The check box for **Other Network File and Print Services** is now white and that one for **Networking Services** grey and both have a tick, click **Next**

7. Click **Start → Control Panel → Administrative Tools → Services**

8. A window '*Services*' will appear:

  a) Scroll down and check the following entries:

  - Simple TCP/IP Services
  - Print Spooler
  - TCP/IP Print Server

  If one of these entries is set to **manual**:

  - Click that entry to highlight it
  - Click **Action → Properties → Startup type →** select **Automatic →** **OK**

9. Click **Start → Turn Off Computer → Restart → Yes**

14.3.2 On the UNIX host from which you want to print

On the UNIX host, you must setup a network printer as follows:

1. Open a UNIX shell

2. Become superuser; type **su**

3. Edit the file /etc/printcap and make an entry like:

```
laserjet|HP :\
:rm=viola.netx.applic.com:\  1
:rp=hplj4ml:\
:sd=/usr/spool/lpd/hplj4ml:\
:sh:
```

---

1. Depending on your network you must enter hostname or hostname.domainname

where:

- *laserjet* is the name for the printer on the UNIX host
- *viola.netx.applic.com* is the hostname.domainname of the PC
- *hplj4ml* is the name of the printer on the PC

4. Create the spooling directory which is specified in `/etc/printcap`:

a) `mkdir -p /usr/spool/lpd/hplj4ml`

b) `chown daemon.daemon /usr/spool/lpd/hplj4ml`

c) `chmod 770 /usr/spool/lpd/hplj4ml`

More information on network printing under UNIX can be found in the manual `netprint` which is available on:

http://www.bruker-biospin.com/documentation_nmr.html

and as '*Network Printing*' in the TOPSPIN online help.

14.4 Installing a printer with a JetDirect print server

If your printer is connected to the network via a HP JetDirect print server, you must install it in the following way:

1. Log in as Administrator

2. Install the Service Microsoft TCP/IP Printing as described in chapter 14.3.1.

3. Click **Start** → **Printers and Faxes**

4. A window '*Printers*' will appear:

- Double-click the icon **Add Printer**

5. A window '*Add Printer Wizard*' will appear:

a) Click **Next** → **Local Printer**, disable '**Automatically detect and install my Plug and Play Printer**', click **Next**

a) Enable **Create New Port** select Type **LPR Port** → **Next**

6. A window '*Add LPR compatible printer*' will appear:

a) In the field **Name or Address of server providing lpd**: enter the name or IP address of the Print Server.

b) In the field **Name of printer or print queue on that server** you must enter:

- **raw1** if you have an internal JetDirect adapter

- **raw1**, **raw2** or **raw3** if you have an external JetDirect print server, depending on the JetDirect port to which the printer is connected.

   c) Click **OK**

7. In the window '*Printer Ports*':

- Click **Close**

8. In the window '*Add Printer Wizard*':

- Click **Next**

9. Continue the installation as described in chapter 14.1.1, step 4d.

Part III

Tips, Tricks and Troubleshooting

Chapter 15

Troubleshooting

15.1 General checks

15.1.1 Windows XP Services

The TOPSPIN requires the following Windows XP Services to control a spectrometer. Proceed as follows:

1. Click **Start** → **Control Panel** → **Administrative Tools**
2. Double-click **Services**
3. A window '*Services*' will appear:

   At least the following services should appear with status **Started**:

   - Bfs
   - Bootparam
   - Bruker FLEXlm License Server (only if the PC has a local license. If the license server is a remote machine, the FLEXlm service has to be started only there)
   - Hummingbird Inetd [1]

---

1. These service is only required for AVANCE and AVANCE-II spectrometers.

- Hummingbird NFS Server [1]
- Hummingbird Port Mapper [1]
- Bruker DHCP Server [2]
- Bruker tftpd32
- Schedule

Note that this list only contains the Services required for the TOPSPIN. Several other Services are required for Windows XP and possibly for other software packages on your system.

4. If one or more of these services are not running:

- Reboot the computer and check again

5. If rebooting does not solve the problem, then proceed as follows:

If bfs and/or bootparam are not running:

- Re-install TOPSPIN and DISKLESS (see chapter 6.4)

If the Hummingbird NFS Server and/or Port Mapper are not running:

- Remove the NFS Server directory

  (normally C:\Program Files\NfsSrvr.nt)

- Re-install the NFS Server (see chapter 4.3)

If the Bruker DHCP Server is not running:

- Please see chapter 15.6

6. Carefully check the NFS Server configuration (see chapter 6.6).

15.1.2 The Event Viewer

If you have any problems on your Windows XP host, it is always a good idea to look at possible Events which caused them:

1. Click **Start → Control Panel → Administrative Tools → Event Viewer**

2. A window '*Event Viewer*' will appear:

- Click **Application Log** to see Application Events
- Click **System Log** to see System Events

---

1. This service has to run only on AVANCE and AVANCE-II spectrometers.
2. This service has to run only on spectrometers with a BSMS rack with ECLB board.

- Click **Security Log** to see Security Events

3. Double-click on an Event to get more information on it.

4. Note that Events do not necessarily indicate problems. If fact, there are three type of events: *Information*, *Warning* and *Error.*

To prevent the Event Log from getting full we recommend to do the following:

5. Click on one of the three Log's, e. g. **System Log** → **Action** → **Properties**

6. A window '*System Log Properties*' will appear:

7. Set the '*When maximum log size is reached*' to one of the following:

- **Overwrite Events as Needed**
- **Overwrite Events Older than 7 Days**

15.2 TOPSPIN does not start

If TOPSPIN does not start, you should first look for an error message in the window where the TOPSPIN startup messages appear. Then check if you have one of the following problems:

1. A window '`Choose Server or File`' appears:

The file `license.dat` was not found. You might have one of the following problems:

- The Flexlm license manager is not installed

  → Install Flexlm license manager from the TOPSPIN CDROM

- `license.dat` has been deleted or renamed

  → Setup the file `license.dat` as described in chapter 7.2.3.

- `license.dat` has a (hidden) extension `.txt` or `.example`

  → Rename the file to `license.dat`

2. If hostid '*0*' or '*ffffffff*' occurs:

You may run Windows XP and your network-adapter has no link to the network. Establish an link to the network or install the

`NWlink IPX/SPX/NetBIOS Compatible Transport Protocol:`

a) Click **Start** → **Control Panel** → **Network Connections**

  b) Right-click **Local Area Connection xxx**

  c) Click **Properties → Install... → Protocol → Add**

  d) The `Select Network Protocol`-menu will appear after some seconds. Click **NWlink ... → OK**

  e) After some seconds the Properties-menu will reappear → Click **Close**

3. '`Cannot connect to license server... WinSock Error code...`'

The file `license.dat` was found, but Flexlm does not run. Maybe:

  a) Flexlm is not installed: → Install Flexlm from the TOPSPIN DVD

  b) the Service (Bruker) Flexlm license server is not running:

      → Click **Start → Control Panel → Administrative Tools**

      • Double-click **Services**

      • A window '*Services*' will appear:

      • Select **Flexlm**..., click **Start**

4. '`Server node is down or not responding (-96,379)`'

The server could not answer because he is down, the entry <SERVER-NAME> in 'license.dat' is wrong or the server has been wrong configured:

      → Check if the server in the 'license.dat' file is down:

      • Click **Start → All Programs → Accessories → Command Prompt**

      • type '**ping <SERVER-NAME>**' and check if the correct reply occurs:

  a) A reply like this:
      `Reply from <SERVER_IP_ADRESS>: bytes=32 time<10ms TTL=128` shows that the server is okay.

  b) A reply like this: '`Request timed out`' shows that the server is down

  c) A reply like this: '`Bad IP address <SERVER-NAME>`' shows that the <SERVER-NAME> is wrong or the server is not correctly configured.

      → Check if the entry of the server in the 'license.dat' file is wrong (wrong name, blanks, ...), if so correct it.

      → Check if the server has a wrong configuration, e. g. TCP/IP protocol or NetBIOS network service is not installed. For this you should have a look at:

      • **Start → Control Panel → Network Connections**

- Click on the LAN entry of your ethernet card → **File** → **Settings**
- A window '*Local Area Connections Properties*' will appear
- Look if there is an entry '*Internet Protocol (TCP/IP)*'
  - Yes? click on it to highlight the entry → **Properties**
  - No? see 13.1.1
- A window '*Internet Protocol (TCP/IP) Properties*' will appear
- Click on **Advanced**
- A window '*Advanced TCP/IP Settings*' will appear
- make sure that the entry '*Enable NetBIOS over TCP/IP*' is enabled

Also click:

- **Start** → **Control Panel** → **Administrative Tools**
- Double-click **Services**
- A window '*Services*' will appear:
  make sure that **server** and **TCP/IP NetBIOS** have the status '*started*'

5. '`Cannot find resolution file`'

  → Reboot the computer and try again

6. '`Invalid license key (inconsistent license key)`'

  The file license.dat might contain one of the following errors:

  - The hostid in the SERVER line is wrong
  - The FEATURE line contains the wrong license key, the wrong date and/or the wrong number of licenses
  - The hostid is appended at the end of the FEATURE line
    (this is correct for *Node Locked* licenses but not for *Floating* licenses, see chapter 7.1)

7. '`Invalid data returned from license server`'

  - Hostname in the file license.dat is incorrect

8. '`Invalid host`'

- The file `license.dat` contains additional characters at the end of the FEATURE line (after ""“")

9. For more information on the Flexlm license manager:

   Click **Start** → **run** enter `c:\flexlm\bruker\help\index.htm` → Click **OK**

10. If you do not get the license to run you can the flexlm_diagnostic.cmd script to send debug information to Bruker BioSpin.:

    1. Double click on the icon 'Bruker Utilities' on the desktop. A window `Bruker Utilities` will appear

    2. Double click on the command prompt

       Note: It is not possible to use a 'normal' windows command prompt, because in this 'special' command prompt of 'Bruker Utilities' there are several parameters and path entries defined.

    3. Enter the command:

       `flexlm_diagnostic.cmd 1>flexlm_diagnostic.out 2>&1`

       The script may require 1 minute to execute.

       Please send the whole output of the TOPSPIN start window using copy&paste and the file *<topspinhome>\flexlm_diagnostic-out.txt* to:

       `nmr-software-support@bruker-biospin.de`

15.3 TOPSPIN troubleshooting

If your current TOPSPIN session has a problem, you can find in this chapter some instructions how to get rid of this situation.

In order to stop TOPSPIN in case of any problems, the first thing to know is, that it is using a client / server structure. It is possible to start more than one client. This feature is used for the remote control but can also be very useful for troubleshooting!

- The client can be stopped without touching a running acquisition.

To get rid of a TOPSPIN problems follow the description below. These steps are increasingly drastic. Please note that this procedure is only necessary in case of any problems as TopSpin does not react anymore.

1. Create debug information and send it to Bruker BioSpin. For this follow the

instructions in chapter 15.3.1

2. Open a Windows command prompt and start a second TOPSPIN graphical user interface with the command:

`<topspinhome>/topspin -client`

`<topspinhome>` is the TOPSPIN installation directory, in a default installation this is `C:\Bruker\TopSpin`

Does the second TOPSPIN graphical user interface works fine?

- Yes? The problem is solved you can go ahead with TOPSPIN.

    Although you can now work with TopSpin you should restart the program as soon as possible. Typically wait until the current acquisition is finished, then exit and restart TopSpin.

- No? go ahead with next step

3. To kill the current TOPSPIN session completely, execute a Windows Command prompt:

`killtopspin`

Note, that this will stop your TOPSPIN session and therefore also a running acquisition.

4. Start TOPSPIN and go on working.

15.3.1 Send debug information to Bruker BioSpin

If you are in a situation, that TOPSPIN problems appear periodically please send information about this to Bruker BioSpin. For a successful and fast processing of incoming emails please make sure that the following information is given:

1. Use TOPSPIN command **`about`** to get the information about:
- version number
- Server patchlevel
- GUI build number

2. Operating system information
- operating system version (Windows Command prompt command **`winver`**)

3. A detailed description how to reproduce the problem

4. TOPSPIN internal debug files. To get these files do the following:

Go into the Windows Command prompt where TOPSPIN was started, maximize

the window and then press the keys **Ctrl** and **Break** simultaneously. This will create a debug output within the Command prompt. To mark the whole text, click with the right mouse button in the Command prompt, a window appears, select **mark all**. Press the keys **Ctrl** and **c** simultaneously. Open a Text Editor (e.g. Notepad).

- click on **Edit → Paste**
- click on **File → Save As...** and enter a name for the file
- click on **File → Exit**

Now it is necessary to pack all available information which Bruker needs to analyze your problem.

Start TOPSPIN and click

   Options → Administration → Execution Protocols → savelogs

or enter in the TOPSPIN command line **savelogs**.

A window Execute Savelogs appears.
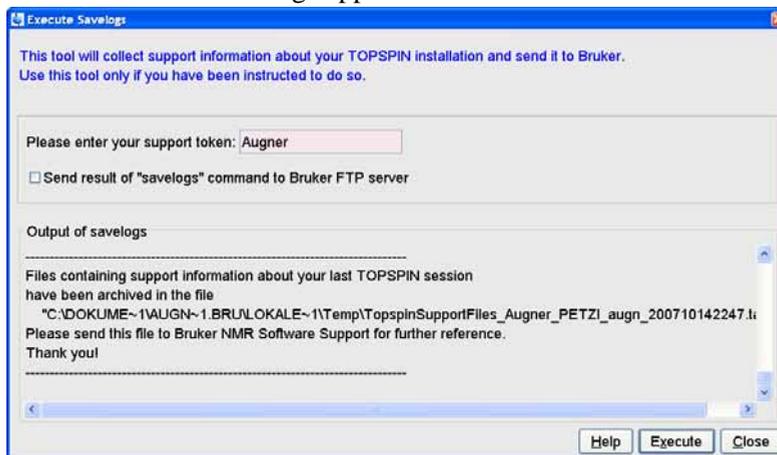
Please enter a support token and click **Execute**.

You can also use the **savelogs.cmd** script which is available under **Bruker Utilities → Miscellaneous**.

Click **Start → All Programs → Bruker TOPSPIN → Bruker TOPSPIN x.y → Bruker Utilities → Miscellaneous.** Double-click the script file: **savelogs.cmd**'. Please enter a support token (e.g. your last name). The script will automatically generate a '*.tar.gz' file with all available debug information from

the TOPSPIN directories. This file will be stored in the directory:

```
<USERHOME>\Local Settings\Temp
```

Please attach these files into an email and send it to this address:

nmr-software-support@bruker-biospin.de

If the file size is too big you can also put it on the german Bruker BioSpin ftp server:

ftp://ftp.bruker.de

You have to login with the user name ‚*ftp*‘ and your email address as password. Now you are authorized to put files into the directory ‚*incoming*‘ (or to get files from the directory ‚*outgoing*‘). When you have uploaded files into ‚*incoming*‘ send an email to

nmr-software-support@bruker-biospin.de

with the information described above and a list of files you have uploaded onto the ftp server.

15.4 Communication problems between PC and Spectrometer

If the acquisition (**zg**, **gs**, **wobb**) and/or configuration (**cf**) fails, you might have a communication problem between the Windows PC and the spectrometer.

Different spectrometer hardware requires different troubleshooting procedures. To find out which spectrometer do you have, check which combination of the following boards are present in your spectrometer.

name	specific boards	Troubleshooting information
AVANCE	CCU-RCU	chapter 15.5
AVANCE-II	CCU-DRU	chapter 15.5
AVANCE-III	IPSO-DRU	chapter 15.6

For a convenient classification the respective boards are shown below. Note, the pictures are just an example, e. g. the EC level can be different.

Do I have an **AVANCE** type spectrometer?

Yes, if you have the two boards:

CCU   *and*   *RCU*

For troubleshooting
information go to
chapter 15.5

CCU11
AQS
ECL 03

RCU1/2
AQS
ECL01

Do I have an **AVANCE-II** type spectrometer?

Yes, if you have the two boards:
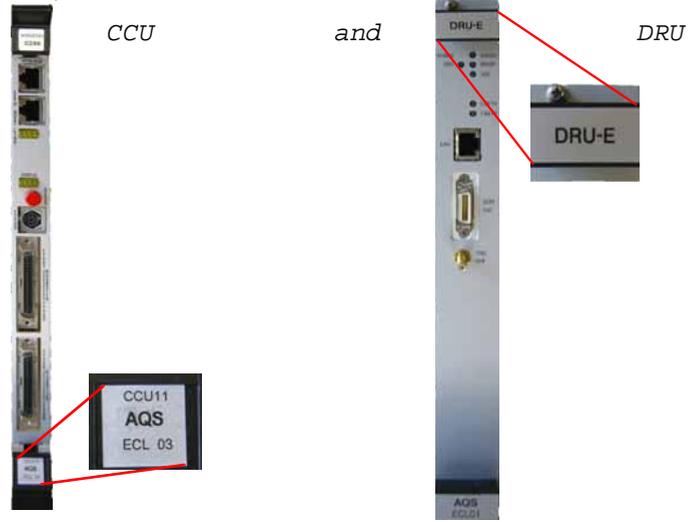
CCU   *and*   *DRU*

For troubleshooting information go to chapter 15.5

Do I have an **AVANCE-III** type spectrometer?

if you have the two boards:

IPSO   *and*   *DRU*
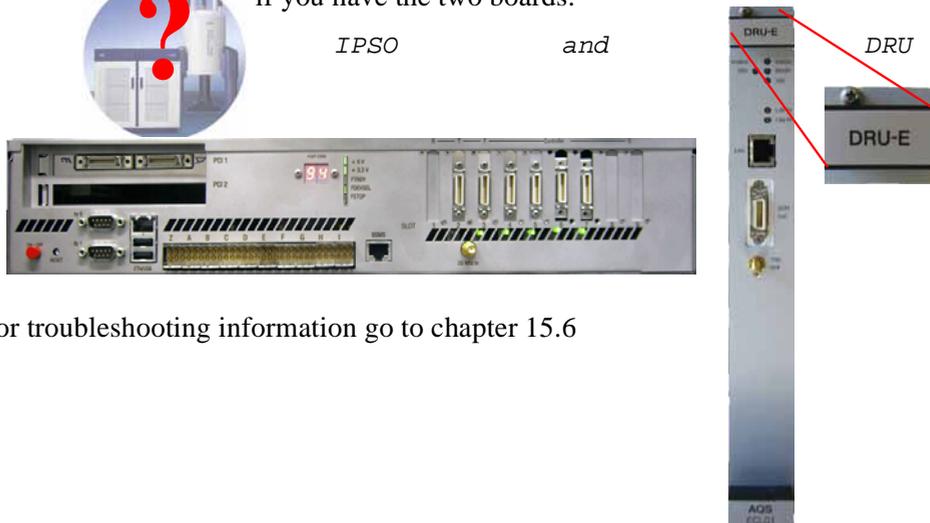
For troubleshooting information go to chapter 15.6

Note: CCU, RCU and DRU have an upright orientation while the IPSO board is typically horizontally orientated.

In all cases the first step of troubleshooting should be to check if the spectrometer is on power and there is a physical network connection between the Windows PC and the spectrometer.

15.5 Troubleshooting for AVANCE and AVANCE-II spectrometers

If the acquisition (**zg**, **gs**, **wobb**) and/or the configuration (**cf**) fails, you might have a communication problem between the PC and the spectrometer CCU. This chapter is for troubleshooting of Avance and Avance-II spectrometers

15.5.1 Hardware related problems

1. Check if the Ethernet cable between the PC and the CCU is properly connected.

→ Remove and re-connect the Ethernet cable.

2. Does the connection light come on if you connect CCU and ethernet board in the PC?

a) If the light is off

The connection light is one of the three LEDs that most Ethernet cards have. One of them, usually in yellow, lights up the same moment that both ends of the respective cable are connected to life devices like a hub or wall socket or a computer.

- Check the cable or the Ethernet card; with some cards you need to reboot the PC with CCU and Ethernet-board being connected to make the initial connection. If the PC is started without any cable connected to the board some configurations will disable the card unless configuration takes place (makes sense for unused cards, however forces us to re-boot more often than we might want to).

- In some cases the auto-negotiate protocol of certain cards doesn't work. That means CCU can't find out whether to go for 10baseT or 100baseT. Some of the newer Ethernet cards allow you to switch the auto-negotiate off. Software configuration allows you to set a fixed speed of 10. In some cases you can also force a card into 10Mbps by putting a hub (a 10Mbps hub!)

between PC and CCU. The hub will tell the card to switch to 10Mbps and CCU gets around auto-negotiate, too.

If the light still doesn't come on, please connect the Ethernet board with some operational network (e.g. corporate network). If you get a physical connection (light goes on) obtain a temporary IP address for the PC and install the card, network, netmask, DNS etc to the point where you see the rest of the company through the 'network neighborhood' of your PC. This will make sure that your card works at all. Then switch back to the IP/netmask for spect and reboot PC. Is the light on? If not, get a new Ethernet card.

b) *If the light is on:*

At this point you know that the physical connection is intact (that is: the connection light on the PC's Ethernet board came on). There are two possibilities to check from here:

- CCU is indeed booting OK, yet you can't access it for some reason.
- CCU really does not boot and you have to find out why.

Before you proceed you might want to quickly check the settings in NFS Maestro. Call it from the Control Panel (HCL NFS Server) and you need to see the configuration given in chapter 6.6. If settings have to be altered, do this, reboot the PC and then the CCU before checking again.

- The minimum test is this: Try to *ping spect* and then to *telnet spect* (see chapter 8.3). Here is how to proceed:

If you can `ping` and `telnet` and get spect's login prompt you should be able to run TOPSPIN from here. You are all set.

If you can `ping` but cannot `Telnet` to CCU the physical connection is all right but CCU doesn't boot. Please connect a monitor cable to CCU and open a Hyper Terminal connection. HyperTerminal is Windows's text terminal emulator and it comes with every copy of Windows. The details are in chapter 15.5.5

If you can't even `ping` CCU try a new Ethernet cable and if it still doesn't work try another type of Ethernet card.

15.5.2 Software related problems

1. Please check if the required Services are running as described in chapter 15.1.1.
2. The firewall may prevent the spectrometer booting. To check this (see chapter 20.8.2):

- Click **Start** → **Control Panel**.
- In the window **Control Panel** → click **Windows Security Center**.
- Click **Windows Firewall**.
  - A window 'Windows Firewall' appears. Click on the **Advanced** tab.
  Yes? No problem, continue with the next step.
  No? You found the problem. Contact your network administrator to correct the firewall settings.

15.5.3 View the output of the CCU console

In order to view the output of the spectrometer CCU, you must connect the COM2 port of the PC to tty00 of the CCU. The hyper terminal application can be used to make the output of the CCU visible on the PC (this has the same function as **cu** and **kermit** on UNIX systems).

15.5.4 Configuration of HyperTerminal

1. Click **Start** → **All Programs** → **Accessories** → **Communications** → **Hyper-Terminal**
2. If you do this for the first time HyperTerminal will ask for some informations in the window '*Location Information*'.Type in your ZIP-code and click **OK**
3. A window '*Phone And Modem Options*' will appear → **OK**

   Then establish a new connection:
4. A window '*Connection Description*' will appear:
   a) In the Field **Icon**: click any icon you decide for
   b) In the field **Name**: enter **CCU**
   c) Click **OK**
5. A window '*Connect to*' will appear:
   a) Click in the field **Connect using**: select **COM2**
   b) Click **OK**
6. A window '*COM2 Properties*' will appear:
   a) Click in the field **Bits per second** and select **9600**
   b) Click in the field **Flow Control** and select **Xon/Xoff**

      (the other settings remain unchanged: Data bits 8, Parity None, Stop bits 1)

c) Click **OK**

→ the output of the CCU will appear in the window '*CCU Hyper Terminal*'

7. Click **File → Save**

8. Click **File → Exit**

9. Answer the question '*Are your sure you want to disconnect now?*' with **Yes**

15.5.5 Usage of Hyper Terminal

1. Click **Start → All Programs → Accessories → Communications → Hypert-erminal → CCU.ht**

2. A window CCU Hyper terminal will appear in which you see the output of the CCU.

If the CCU is booted, you will see a login prompt and you can log in as root. If the CCU is not booted you can push the reset button on the CCU and view the boot process. The boot process is shown below. The messages '*Fast ethernet...*' only occur for CCU/9 and indicate whether you have a 10 MBit/s or 100 MBit/s ethernet connection. Note that a UNIX pathname for the DISKLESS program is shown. Do not worry about this, it is automatically interpreted as an Windows XP path like: C:\Bruker\Diskless...

```
Autoboot:   Waiting   to   load   bfs()/usr/diskless/cli-
ents/spect/root/unix.r4600_std (
CTRL-C to abort)
loading


Fast ethernet (FEN): 100 MBit/s, half duplex
    ---1---
Obtaining  /usr/diskless/clients/spect/root/unix.r4600_std
from server 'hostname'
833328+107984+827152 entry: 0x80021000
CPU: MIPS .... Processor Chip Revision: ...
FPU: MIPS .... Floating Point Unit [CP1] Revision: ...

RISC/os Release 4_52 mips Version UMIPS
Total real memory = 16777216
Available memory  = 14360576
Root on nfs file :,Swap on nfs f
Fast ethernet (FEN) : 100 MBit/s, half duplex
```

```
   ---2---
hostname: spect
domainname: software.bruker.de
   ---3---
Root fstype nfs
Available memory  = 12713984


   ---4---
The system is coming up. Please wait.
/etc/init.d/sym_install start
/etc/init.d/sym_install calls sym_install
Adding swap device /swapfile
Fast ethernet (FEN) : 100 MBit/s, half duplex
Internet daemons: portmap inetd.
NFS daemons: nfsd biod lockd statd.
/tmp: Permission denied
/var/tmp: Permission denied
The system is ready:


spect Console login:
```

Booting might hang, stop (and print an error message) or go into an endless loop at one of the positions 1 through 3. This might be caused by one of the problems mentioned below. Check the indicated files and correct them if necessary or perform the indicated steps.

a) If booting stops at position ---1--- and you get the messages:

```
Fast ethernet (FEN): 100 MBit/s, half duplex
No  server  for  /usr/diskless/clients/spect/root/un-
ix.r4600_std
BRUKER CCU R4600 Monitor
Version 5.40 MIPS OPT Wed Jun 11 19:30:43 MSZ 1997 root
Memory size: 16777216 (0x1000000) bytes, 16 MB
Icache size: .... (....) bytes
Dcache size: ..... (....) bytes

>>
```

then you might have one of the following problems:

- The Service *bfs* not running:

    Click **Start → Control Panel → Administrative Tools → Services → bfs → Start**

- The Diskless package is not installed (see chapter 6.4)
- The ethernet cable between PC and CCU allows no data throughput:

    - check the connection between the cable and the PC/CCU

    - check if the correct ethernet card is connected

    - check the configuration of the ethernet port (see chapter 13.1)

b) If booting stops at ---2--- you may have one of the following problems:

- The Service *bootparam* is not running:

    Click **Start → Control Panel → Administrative Tools → Services → bootparam → Start**

- The file `C:\Windows\system32\drivers\etc\Hosts` is wrong:

    It should contain the following entries:

    ```
    149.236.99.1 ASP_ST2
    149.236.99.99 spect
    ```

    Be sure that 'spect' is the first entry after the number in this line

- Be sure that the spectrometer ethernet card is configured for 'half duplex'.
    Click **Start → Control Panel → Network Connections →** select the spectromter ethernet card → click **Properties →** click **Configure →** select **Advanced →** select **Speed & Duplex →** change the value to **100 Mb Half Duplex**

c) If booting stops at ---3--- you might have the following problem:

- The file `c:\Bruker\Diskless\WinApp\bootparams` is wrong.
    For a default installation it must contain the lines:

    ```
    #
    spect  root=ASP_ST2:C:/Bruker/Diskless/clients/spect/root \
          swap=ASP_ST2:C:/Bruker/Diskless/clients/spect/swap \
          dump=ASP_ST2:C:/Bruker/Diskless/clients/spect/dum
    ```

    For a custom installation the path of Diskless can be different!

d) If booting hangs at ---3--- in a loop and you get the messages:

a) like this:

    ```
    domainname: software.bruker.de
    mount  root  ASP_ST2:C:/Bruker/Diskless/clients/spect
    ```

```
/root failed, rpc status 15
PANIC: vfs_mountroot: cannot mount root
syncing disks... done
```

then you might have one of the following problems:

- The Service Hummingbird NFS Server is not running

  Click **Start** → **Control Panel** → **Administrative Tools** → **Services** → **Hum. NFS Server** → **Start**

- The path `C:\Bruker\Diskless\clients\spect` is not exported (see chapter 6.6).

b) like this:

```
domainname: software.bruker.de
mount  root  ASP_ST2:c:/Bruker/Diskless/clients/spect
/root failed, rpc status 2
PANIC: vfs_mountroot: cannot mount root
syncing disks... done
```

then you might have the problem that the drive letter of the diskless installation is written in lower case (maybe caused by a custom installation). To solve the problem you can either

- De-install Diskless and use for the new installation '*typical*' or make sure that the drive letter is upper case

or

- Open the file

  `c:\Bruker\Diskless\WinApp\bootparams`

  and change all drive letters to upper case

c) If booting stops at ---4--- and you get messages like this:

```
<date> INIT: Can't open /etc/ioctl.syscon. errno: 13
touch: /etc/mtab cannot create
mount: /etc/mtab: No such file or directory
<date> INIT: warning: /etc/ioctl.syscon does not ex-
ist, default settings assumed
<date> INIT: Can't open /etc/ioctl.syscon. errno: 13
<date> INIT: Cannot create /etc/utmp
<date> INIT: failed write of utmp entry: "    "
```

Please check diskless tree permissions and NFS User- and Group-Map-

pings (see Chapter 6.6)

d) If you see the message:

mount dumpfile ASP_ST2:C:/Bruker/Diskless/clients/spect/dump failed

during the boot process, you can ignore this. The CCU will boot anyway.

3. Click **File** → **Exit** to finish your Hyper Terminal session.

15.6 Troubleshooting for AVANCE-III type of spectrometer

There are some differences in troubleshooting AVANCE / AVANVCE-II and AVANCE-III type of spectrometers. An important difference is, that on AVANCE-III spectrometer is neither **telnet spect** available nor a nfs server necessary. Several hardware units are connected via ethernet devices and controlled via a DHCP Server. This DHCP server comes with the Diskless installation of the TOPSPIN DVD. The process is called *Bruker DHCP Server*.

To find out what are the IP addresses of the different (via ethernet connected) hardware units there are two different possibilities:

- the TOPSPIN command **ha** (for **h**ardware **a**ddresses)
- the command **ethernet-service-tools**

Both commands offer a list of available (via ethernet connected) hardware units and their IP addresses. A mouse click on the name of a module opens the start page of the respective module in a web browser. From there it is easy possible to reset, test and configure the hardware unit. The firmware download can also be started from there.

Note: The web pages of the hardware units are optimized for the web browser Microsoft Internet Explorer.

15.6.1 Communication problems with an AVANCE-III spectrometer

To check if an AVANCE-III is booted correctly you can use the following tests:

1. To check which ethernet connected hardware units are available you can use one of the two commands **ha** or **ethernet-service-tools**

- TOPSPIN command **`ha`**
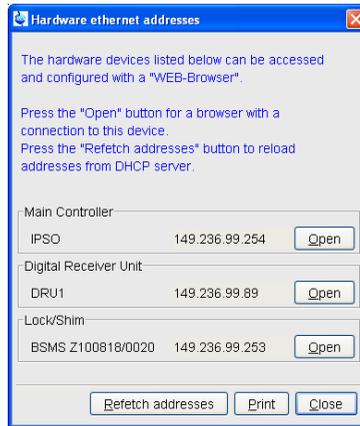
A window appears that shows several hardware modules. Does the window offers an entry for the Main Controller?

Yes? The AVANCE-III is booted correctly, go on with the TOPSPIN command **`cf`**

No? Go to step 2

- Open **Command Prompt** (Click **Start** → **All Programs** → **Bruker TOP-SPIN** → **Bruker TOPSPIN x.y** → **Bruker Utilities** → **Command Prompt**) and enter the commands:
  - **`cd prog/bin`**
  - Click **Enter**
  - **`ethernet-service-tools`**
  - Click **Enter**

A window appears that shows several hardware modules. Does the window

offers an entry 'IPSO'?
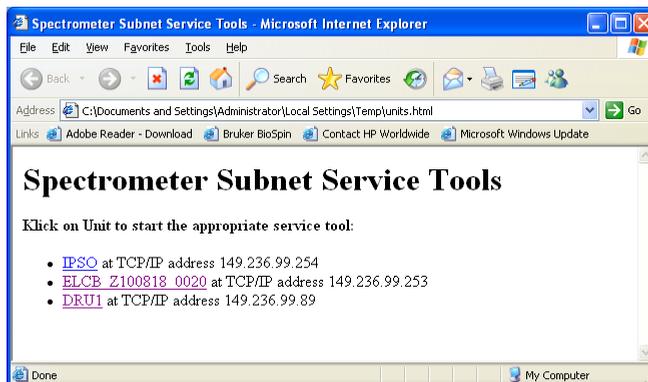
Yes? The AVANCE-III is booted correctly, go on with the TOPSPIN command
`cf`

No? Go to step 2

2. Check the network configuration:

   a) Check the network configuration according the information in chapter 13.1.

   b) Check the file `C:\WINDOWS\system32\drivers\etc` - at least the following entries have to exist for spectrometer control:

   127.0.0.1   localhost.localdomain   localhost

   149.236.99.1   ASP_ST2

   149.236.99.99   spect

   If the ethernet card for the laboratory network is not configured as DHCP, also the name of the own PC has to be listed

   xyz.xyz.xyz.xyz   name_of_own_pc.domain   name_of_own_pc

   Does this entry exists?

   Yes? No problem, continue with the next step.
   No? You found the problem. Add the name of the PC as described in chapter 13.2. Then reboot the PC and check if the spectrometer now boots correctly.

   c) Check if the hostname and IP address of the PC is correctly available in the nameserver.

   • open a Command Prompt

- type in **ipconfig /all**

    The entries should look like this:

    Yes? No problem, continue with the next step.

    No? You found the problem. Contact your network administrator to correct the settings.

3. The firewall may prevent the spectrometer booting. To check this (see chapter 20.8.2):

    - Click **Start** → **Control Panel**.

    - In the window **Control Panel** → click **Windows Security Center**.

    - Click **Windows Firewall**.

        - A window 'Windows Firewall' appears. Click on the **Advanced** tab.

        Yes? No problem, continue with the next step.

        No? You found the problem. Contact your network administrator to correct the firewall settings.

4. The DISKLESS package is not installed. Insert the TOPSPIN DVD into the DVD drive, select the DISKLESS package and de-select all other packages. For more details see installation description in chapter 6.4. After installation of DISKLESS reboot the spectrometer.

5. Check if the Bruker DHCP Server is running.

- Open a Command Prompt and enter the command

    net start

    Under '*These Windows services are started*' has to be mentioned:

    Bruker DHCP Server

    Yes? The DHCP service is running, go to the next step

    No? You may have found the problem, the Bruker DHCP Server is not running, try to start them with:

    a) Click **Start** → **Control Panel** → **Administrative Tools**

    b) Double-click **Services**

    c) A window '*Services*' will appear:

      Select the service: **Bruker DHCP Server**

    d) Right-mouse-click on this service and select **Start**.

    Now you have to reboot the spectrometer.

    Yes? The service is running, go to the next step

    No? You may have found the problem, the Bruker DHCP Server cannot be started.

6. Change the binding of the *spect* ethernet card:

    a) Log in as Administrator

    b) Click **Start** → **Control Panel** → **Network Connections**

    c) A window '*Network Connections***'** will appear

      Highlight the connection which is configured for the IP-adress

149.236.99.1
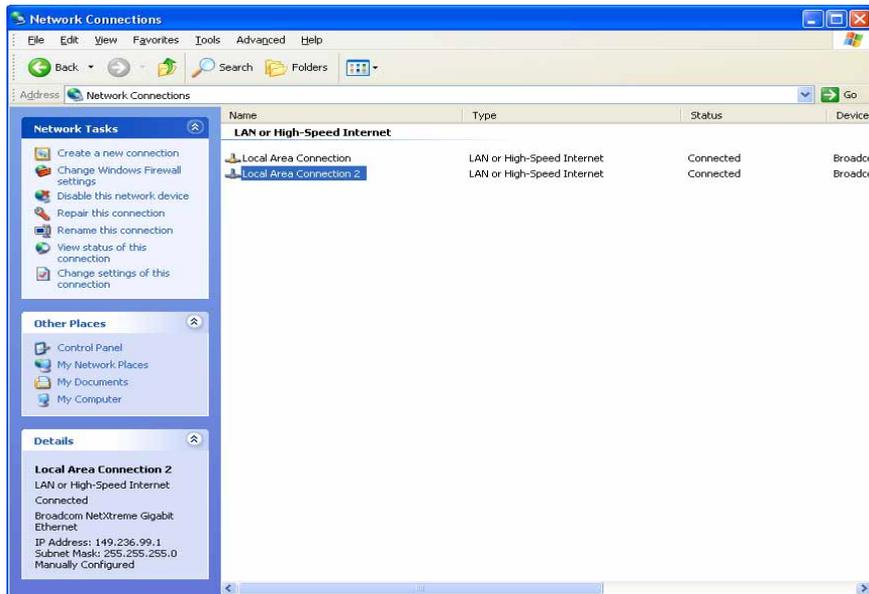
Right-mouse-click on this connection and select **Rename** and rename it to *spect*
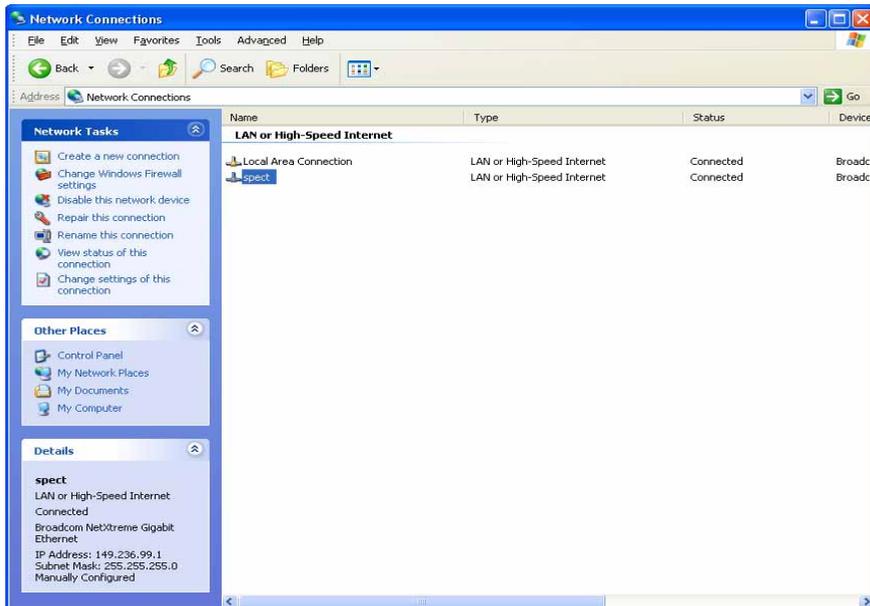
d) Click **Advance** → **Advance Settings...**

A window '*Network Connections*' will appear
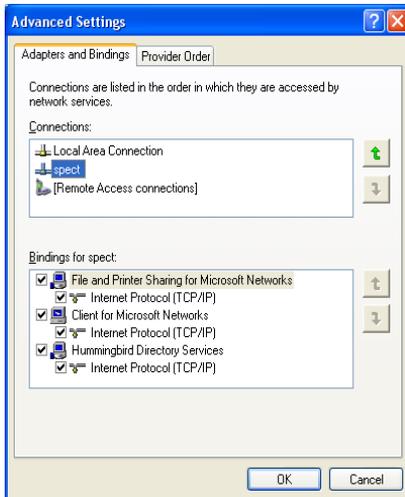
e) Please check if the *spect* entry is on the second position.

f) If not please move the entry with the arrow buttons on the right side of the window to the second position.

g) Click **OK**.

Yes? The service can be started, go to the next step

No? You may have found the problem, the Bruker DHCP Server cannot be started:

7. Swap the functions of the two ethernet cards (spect and network) between them:

a) Log in as Administrator

b) Click **Start** → **Control Panel** → **Network Connections**

c) A window '*Network Connections*' will appear

d) Highlight the connection you want to configure (It is recommended to change first the settings for the ethernet card which is configured for the IP-adress 149.236.99.1). Click **File** → **Properties**

e) Highlight the TCP/IP entry and click **Properties**

Change the entries.

    f) Repeat the handling for the second ethernet card.

    g) Reboot the PC.

Note: Do not forget to swap the ethernet cables (!) and to reboot the PC!

Yes? The service can be started, go to the next step

No? You may have found the problem, the Bruker DHCP Server cannot be started:

8. Check if the Bruker tftpd32 is running.

- Open a Command Prompt and enter the command

    `net start`

    Under '`These Windows services are started`' has to be mentioned:

    `Bruker tftpd32`

Yes? The tftpd32 service is running, go to the next step

No? You may have found the problem, the Bruker tftpd32 is not running, try to start them with:

    a) Click **Start → Control Panel → Administrative Tools**

    b) Double-click **Services**

    c) A window '*Services*' will appear:

       Select the service.: **Bruker tftpd32**

    d) Right-mouse-click on this service and select **Start**.

Now you have to reboot the spectrometer.

If these troubleshooting steps do not give any hint on an existing problem, you might have a hardware problem. Please get in contact with your local Bruker BioSpin office. Adresses of several offices can be found in chapter 22, for contact information about all Bruker BioSpin office please go to our web server:

http://www.bruker-biospin.com/contact_us.html

15.7 Troubleshooting for NMR-GUIDE

If you have some trouble with your installation of the NMR-GUIDE, please check

the following :

1. Check for the NMR-GUIDE license (see chapter 7)

   Edit the file `C:\flexlm\Bruker\licenses\license.dat` and check weather there is a FEATURE NMRGUIDE line. If not, enter the FEATURE line or apply for a license at

   license@bruker.de

2. Check for all necessary components
   - Internet Explorer $\geq$ 6.0 (see chapter 3)

3. Install the NMR-GUIDE program from the TOPSPIN DVD once again and reboot. (This is necessary, because installation of the operating system components might have overwritten certain registry keys that are set during the NMR-GUIDE installation.)

4. Now try the NMR-GUIDE again

15.8 helium measurement not startet

If the helium measurement will not be started please check in the directory

`<topspinhome>\prog\logfiles`

the two files `heliumlog` and `heliumlog.err`. The `heliumlog` file include the values according the helium measurements. If an error occurs during the measurement this will be reported in `heliumlog.err` file.

If both files are empty please try to set up a new sheduled task.

Create a new "Scheduled Task" to start the helium measurement:

1. Login as local administrator.

2. Click **Start** $\rightarrow$ **Control Panel** $\rightarrow$ select **Scheduled Tasks**

3. Click on "Add Scheduled Task"

4. A window "Scheduled Task Wizard" appears $\rightarrow$ click *next*

5. In the appearing window click on the *Browse* button and go to

`<topspinhome>\prog\bin` (e.g. `C:\Bruker\TOPSPIN\prog\bin`) and select `helevtransfer.cmd` and click *open*

6. In the next window select under 'Perform this task' the option 'Daily' and click *next*

7. Select for 'Start time' "03:00 AM" and 'Perform this task' "Every Day" → click *next*

8. In the next window click on *next → finish*

15.9 Bruker Service tools

Several tools for checking the spectrometer hardware are delivered with TOPSPIN. This includes tools for BSMS, HPPR, ACB, GRAD, HPCU, RX22. You can start a service tool as follows, for a full description see chapter 8.6:

1. Double-click the icon **Bruker Utilities** on the desktop

2. A window will appear with the icons Service tools, Test Tools etc.:

  a) Double-click **Service Tools** to get a list of service tools

  b) Double-click **Test tools** to get a list of test tools

3. A windows with the available tools will appear:

  • Double-click any icon to start the corresponding tool

15.10 Windows XP Service Pack

All PC's delivered by Bruker BioSpin have the latest Service Pack installed. It can also be downloaded from the Microsoft Web pages `www.microsoft.com` or `www.microsoft.de`.

For installation just follow the given instruction on the screen.

Under Windows XP it is not necessary to reinstall the service pack after e. g. configuring the network.

During the installation, you might get the message that files were detected which are not the original Windows XP files and which are also part of the Service Pack. Sometimes, these files are even newer than the ones in the Service Pack. This typically happens when you installed recent driver software. You are asked if these files should be overwritten. Bruker BioSpin recommends to answer this question with **No**, unless you are sure you want to update this file from the Service Pack.

15.11 Disk full or fragmented

If you have disk space problems, have a look at the Windows XP Online help:

Click **Start** → **Help** → **Index**

enter `increasing disk space` choose one subentry and click **Display**. If you want to defragment your disk see chapter 19.3. Note that NTFS partitions, which are required for TOPSPIN, suffer much less from fragmentation than FAT partition.

Furthermore, you might have to remove TOPSPIN data, e.g.:

1. Delete imaginary data using the `deli` command

They are no longer needed for spectra which have been phase corrected.

2. Delete processed data using the `delp` command

They can always be retrieved by reprocessing the data.

3. Delete raw data with the `del` command

Please make sure you have a backup of the data.

15.12 Creating an Windows XP Boot Disk

You can use a Windows XP bootable disk to start the operating system on a computer running Windows XP. Use the procedures in this article to work around the following boot issues:

- Damaged boot sector.
- Damaged master boot record (MBR).
- Virus infections.
- Missing or damaged ntldr or ntdetect.com files.
- Incorrect ntbootdd.sys driver.

You cannot use the Windows XP boot disk to help resolve the following issues:

- Incorrect or damaged device drivers that are installed in the System folder.
- Boot issues that occur after you see the Windows XP startup (Osloader) screen.

15.12.1 PC is not booting from floppy?

In case it is not possible to boot the PC from a bootable floppy, this possibility might be disabled in BIOS. The following description shows how to enable the boot-from-floppy feature on a hp workstation xw4400 PC. On other PC's the procedure might be slightly different.

1. During boot time cancel the boot process and go into BIOS

   On different PCs there are different ways to do this, for example, on some PCs the boot sequence is interrupted with the **Delete** key rather than with the **F2** key.

2. Go to section

   Security → Boot Devices Security

3. Set *Floppy* to **Enabled**

Note: It is recommended to disable the boot-from-floppy feature after the boot process is done!

If it is enable, it is possible to get very easily a boot virus into BIOS, that can make your PC defective!

Another small advantage is, that if the BIOS feature above is enabled and a 'normal' floppy is inside the drive, booting the PC will stop and showing the information that a non bootable floppy is inside. If it is disabled booting the operating system will work with or without floppy.

15.12.2 Floppy boots Operating System from hard disk

You can create an Windows XP Boot Disk by formatting a floppy from within Windows XP and copying the following files from the root of an Windows XP boot partition (e.g. C:) to the floppy (Special note: the boot partition is the first partition which is read by bios. This is normally but not necessary the partition 'c:'. If you installed Windows XP on a different partition e.g. 'd:', the following files are anyhow on 'c:'.

- `ntldr`
- `ntdetect.com`
- `boot.ini`

If you are using SCSI disks with the SCSI BIOS <u>disabled</u> then also copy the file:

- `ntbootdd.sys`

a) Create a Boot Floppy Disk with the command prompt

Copy these files with command prompt is easier to describe than with the Windows explorer, because these are critical system files that are normally not shown in the explorer window.

1. Click **Start → All Programs → Accessories → Command Prompt**
2. Type **`c:`**
3. Type **`dir /ah`** → you should see the necessary files
4. Type **`xcopy /h boot.ini a:`**
5. Type **`xcopy /h ntldr a:`**
6. Type **`xcopy /h ntdetect.com a:`**
7. If necessary (see above) type **`xcopy /h ntbootdd.sys a:`**

Now you can boot your PC from the Boot floppy. Be aware that this will only work if Windows XP is still on the hard disk. If Windows XP is not available or corrupt it must be repaired again from CDROM or from floppy.

b) Create a Boot Floppy Disk with the Windows Explorer

1. Format a floppy disk by using the Windows XP format utility.
2. Copy the `ntldr` and the `ntdetect.com` files from the I386 folder on the Windows XP Setup CD-ROM, Windows XP Setup floppy disk, or from a computer that is running the same version of Windows XP as the computer that you want to access with the boot floppy.
3. Copy the `boot.ini` file from a computer that is running Windows XP. Or create a `boot.ini` file, and then modify it to match the computer that you are trying to access. The following example works for a single-partition IDE drive with Windows XP installed in the \Windows folder, but the exact value in the [operating systems] section depends on the configuration of the Windows XP computer that you are trying to access:

```
[boot loader]
timeout=30
Default= multi(0)disk(0)rdisk(0)partition(1)\windows

[operating systems]
multi(0)disk(0)rdisk(0)partition(1)\windows="Windows XP"
```

If your computer boots from a SCSI hard drive, you may need to replace the multi(0) entry with scsi(0). If you are using scsi(x) in the `boot.ini` file, copy the correct device driver for the SCSI controller in use on the computer to the root of the Setup disk, and then rename it `ntbootdd.sys`. Change the disk(0) number to represent the SCSI-ID of the hard drive you want to boot to. If you are using multi(x) in the `boot.ini` file, you do not need to do this.

4. Start your computer by using the floppy disk, and then log on to Windows XP.

15.13 Backup of Windows XP and TOPSPIN

The standard backup programs under Windows XP is called **ntbackup** which can be started by clicking:

Start → All Programs → Accessories → System Tools → Backup

Under Windows XP ntbackup is possible to use ZIP, tape and external hard disks as backup media.

You cannot choose a CD-R, CD-RW, or DVD-R device because ntbackup.exe does not support backing up to these devices. The **R**emovable **S**torage **M**anagement (RSM) does not have the ability to recognize these three devices as backup pool media. RSM regards CD-R, CD-RW, or DVD-R as just a file system-capable media type, but the Windows file system does not support formatting these media types. When it attempts to write an RSM free label, RSM does not succeed because the disc appears to be write protected. This means that RSM treats CD-R, CD-RW, or DVD-R media as a read-only media type even if you add them to the ntbackup media pool. Before you buy a tape drive, make sure it is compatible with your PC's interface(s); IDE and/or SCSI.

Bruker BioSpin recommends to make a regular backup of the partition(s) on which Windows XP and the TOPSPIN are installed.

15.13.1 Complete Backup of the PC

1. Click **Start → All Programs → Accessories → System Tools → Backup**

→ a window *backup* will appear

2. Click **Welcome → Backup Wizard**

$\rightarrow$ a window *Backup Wizard* will appear $\rightarrow$ **Next**

3. Enable *Backup everything on my computer* $\rightarrow$ **Next**

4. Choose the media drive you want to store the backup $\rightarrow$ **Next**

5. Click '*Finish*' to start the backup

15.13.2 Backup of specific directories

1. Click **Start** $\rightarrow$ **All Programs** $\rightarrow$ **Accessories** $\rightarrow$ **System Tools** $\rightarrow$ **Backup**

$\rightarrow$ a window *backup* will appear

2. Click **Backup**

$\rightarrow$ all available drives will appear

3. Choose the directory you want to backup. Click the check box left of the directory to select the entire path for backup $\rightarrow$ a tick will appear in the check box

4. Choose the *Backup media or file*

5. Click **Start Backup**

6. A window *Backup Job Information* will open

7. Click **Start Backup**

15.13.3 Frequent backup of specific directories

If you commonly use Ntbackup to back up a single folder, you might want to create a simple batch file. Suppose you would like to make a daily backup of a directory:

1. Choose the path of the file as describe above

2. Click **Start Backup**
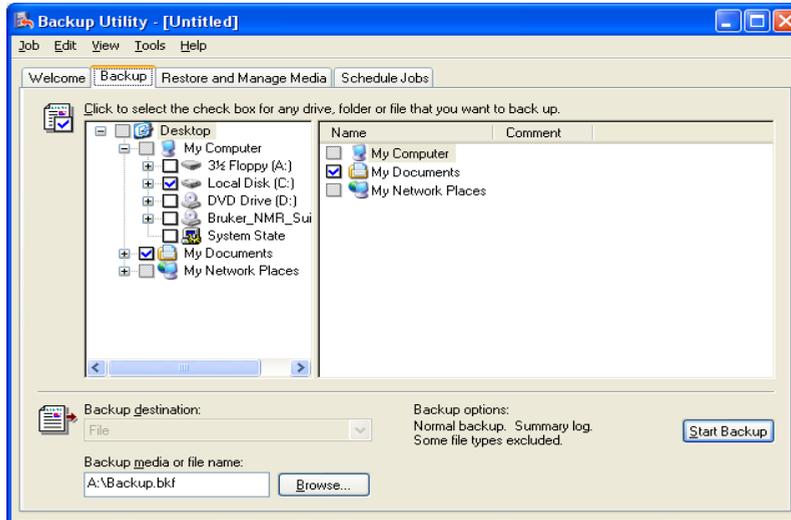
3. A window *Backup Job Information* will open

4. Click **Advanced**
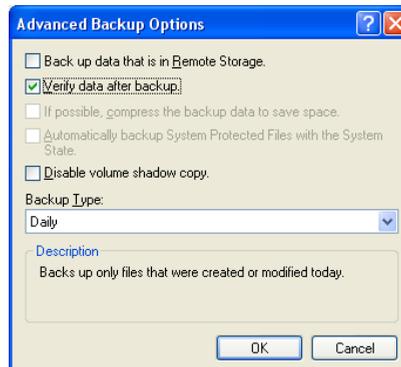
5. Click the arrow at the right of the field *Backup Type* and choose **Daily**

6. Click **OK** → Click **Start Backup**

15.14 Security check of a Windows XP system

Microsoft offers a tool for free download that checks your PC for security leaks. The result is listed with an evaluation of the different topics. For further details check the following Microsoft website.

```
http://www.microsoft.com/technet/treeview/default.asp?url=/tech-
net/security/tools/Tools/mbsahome.asp
```

15.15 Restore the Operating System to a Previous State in Windows XP

Use the System Restore tool in order to return your computer to a previous working state. The System Restore takes a 'snapshot' of critical system files and some program files and stores this information as 'restore points'. You can use these 'restore points' to return Windows XP to a previous state.

15.15.1 Using System Restore to Restore Windows XP

- **Windows XP Does Not Start**

  If Windows does not start, restart Windows by using the 'Last Known Good Configuration' feature:

  1. Start the computer and then press the **F8 key** when Windows begins to start. The 'Windows Advanced Options' menu appears.

  2. Select 'Last Known Good Configuration' (your most recent settings that worked), and then press **ENTER**.

  3. If a boot menu appears, use the ARROW keys to select **Microsoft Windows XP**, and then press **ENTER**. Windows XP restores the computer to the most recent restore point.

- **Windows XP Does Start**

  1. Log on to Windows as an administrator.

  2. Click **Start** → **All Programs** → **Accessories** → **System Tools** → **System Restore**. System Restore starts.

3. A window *Welcome to System Restore* appears, click **Restore my computer to an earlier time** (if it is not already selected) → click **Next**.

4. A window *Select a Restore Point* appears. Click the most recent system checkpoint in **On this list**, click a **restore point** list → click **Next**.

5. A System Restore message may appear that lists configuration changes that System Restore will make → click **OK**.

6. On the Confirm Restore Point Selection page, click **Next**. The System Restore will restore the previous Windows XP configuration and then restarts the computer.

7. Log on to the computer as an administrator. A window *The System Restore Restoration Complete* will appear → Click **OK**.

15.15.2 Troubleshooting

It could happen that you restore Windows XP to a previous configuration that you do not want. To undo the restoration:

1. Log on to Windows as an administrator.

2. Click **Start** → **All Programs** → **Accessories** → **System Tools** → **System Restore**. System Restore starts.

3. A window *Welcome to System Restore* appears. Click **Undo my last restoration** → **Next**.

4. A System Restore message may appear that lists configuration changes that System Restore will make → click **OK**.

5. On the **Confirm Restoration Undo** page, click **Next**. System Restore restores the original Windows XP configuration, and then restarts the computer.

6. Log on to the computer as Administrator. A window *The System Restore Undo Complete* appears → Click **OK**.

15.16 Turn on and turn off System Restore in Windows XP

The 'System Restore' is the feature that allows a computer system to be 'rolled back', or restored, to a point in time before certain events took place, for example, prior to specific software or hardware installations. System Restore monitors changes to the system and some application files, and automatically creates restore points. You can also create your own restore points at any time.

In Windows XP the 'System Restore' is enabled by default.

15.16.1 Turn on System Restore

To turn on System Restore, follow these steps:

1. Click **Start** → right-click **My Computer** → click **Properties**.
2. Click the **System Restore** tab.
3. Click to clear the **Turn off System Restore** check box (or the **Turn off System Restore on all drives** check box) → click **OK**.

15.16.2 Turn off System Restore

When you turn off System Restore, all existing restore points are removed, and you are no longer able to track or undo changes to your computer. To continue to use System Restore to restore your computer to a previous state, do not turn off System Restore.

To turn off System Restore, follow these steps:

1. Click **Start** → right-click **My Computer** → click **Properties**.
2. Click the **System Restore** tab.
3. Click to select the **Turn off System Restore** check box (or the **Turn off System Restore on all drives** check box) → click **OK**.
4. Click **Yes** when you receive the prompt to the turn off System Restore.

15.17 Start the system restore tool from a command prompt in Windows XP

Windows XP includes the System Restore tool, but you cannot start the System Restore tool from a Recovery Console prompt. Because of this, it may be useful to start the System Restore tool when you are unable to start your Windows XP-based computer normally or in Safe mode.

NOTE: You must log on with administrator rights.

1. Start your computer to Safe Mode with Command Prompt.
2. At the command prompt, type

   ```
   %systemroot%\system32\restore\rstrui.exe
   ```

and then press ENTER.

Follow the instructions on the screen to begin restoring your computer to a previous, functional state.

15.18 Logon problems: Last Known Good

Changes in the Registry must be made with extreme care, any mistakes can make the system unusable. Occasionally, software installations make erroneous Registry entries. If your PC does not boot any more, you can try to go back to the so-called Last Known Good, the last Registry Control Set with which the system successfully booted. Please proceed as follows:

1. Reboot and Interrupt the boot process hitting F8 when you see:

For troubleshooting and advanced startup of Windows XP press F8

2. Use the arrow down/up keys to select the entry '*Last Known Good*', then press **ENTER** and follow the instructions

Warning: when you reboot the computer after you installed new software, wait until all disk activity has finished, before you log on. As soon as you log on, the current control set becomes the Last Known Good and the Original Control Set (before software installation) is gone.

15.19 The Emergency Recovery DVD

Each PC which is delivered from Bruker BioSpin Germany comes with a Emergency Recovery DVD. This DVD contains an image of the PC and can be used for restoring the PC. The image contains the installed and pre configured operating system and all necessary programs like TopSpin. It does not contain any user specific data, like spectrometer configuration, NMR datasets or network configuration.

In case of a hard disk crash, a hacked system, or even a stolen PC it is possible to get back on a new PC hardware a well working system within 20 minutes. After restoring the image the last nmr_backup file must be restored and the TopSpin command *cf* must be executed.

More information about nmr_backup and the TopSpin command *nmr_save* file are available in chapter 8.8

15.19.1 Using the Emergency Recovery CD

! Note: This should be done by experienced people only! All data currently on the disk will be destroyed!

● If in doubt please contact your system administrator, maybe it is still possible to get data from the old disk. New hardiest are not expensive therefore using a new hardiest for restoring an image might be the best solution!

1. Insert the *Bruker Emergency Recovery DVD* and boot the PC. The window *Image Boot DVD Bruker Biospin* will appear.

   → Press **F1**

2. The *Acronis True Image* selection window appears

   Select *Acronis True Image (full version)*

   Acronis True Image will be started. This will take about 2 minutes.

3. The window *Acronis True Image* appears.

   → Click on **Recovery**

4. The window *Welcome to the Restore Image Wizard* appears.

   → Click on **Next**

5. In the window *Image Archive Selection* click on the plus sign left to *CD Drive*. Typically this is (D:) or (E:). You will see some directory and disk icons.

   → Click on the first disk icon below the directory icons.

   On the right side a short description of the image DVD will appear. Please read this carefully and make sure that this is the image you like to install on this PC.

6. Click **Next** in the window *Restored Hard Disk Drive Location*

7. Select the hard disk on which you want to restore the image. In general you will have only one hard disk available, so click on this line and then click **Next**.

8. In the window *Verify Archive Before Restoring* you can verify the image before it is used. This would need the same time which is necessary for restoring the image.

9. In the window *Partition or Disk to Restore* check the box left to *Disk 1* to restore the complete image.

10. In the window *Restore Partitions Resize* you now have the possibility to change the size of individual partitions. This is only necessary e. g. if you use a smaller hard disk that on which the image was created. So if you use the same disk size

you can check *No, I do not want to resize partitions.*

→ Click on **Next**

11. In case the hard disk which you have selected contains already partitions you must select *Yes, I want to delete all the partitions on the destination hard disk drive before restoring.*

→ Click on **Next**

12. In the window *Next Selection* select *No, I do not* because you only want to restore the image on one hard disk.

→ Click on **Next**

13. In the last window you will get a summary of the chosen operations. Check if everything is defined correctly.

→ Click on **Proceed**

14. Restoring image will then be started. This process will take about 20 minutes. When it is finished a window will appear with information *Image was successfully created.*

15.20 An image of the PC

Each PC which is delivered from Bruker BioSpin Germany has a license for the backup tool *Acronis True Image.* With this software it is possible to create a one-to-one backup of the hardiest of the system.

It is recommended to periodically create a backup of the hardiest. In case of any problems (hardiest crash, virus, hacker attack ...) you are able to rebuild the situation of your last backup within a few minutes.

In chapter 15.19 it is described how to use the Bruker Emergency Recovery DVD. This DVD contains the first image of the PC. If you create periodically a new image of your PC you will be able to restore a system which is much more up-to-date and contain all your individual settings like network configuration, user management, spectrometer configuration etc.

15.20.1 Creating an image

You need a boot-CD to start Acronis True Image, if there is no such CD, you can install Acronis True Image on a Windows system and create the *Bootable Rescue Media* from there. The original *Acronis True Image installation CD* is usually

bootable.

1. Insert a bootable Acronis True Image CD and boot the PC. The window *Acronis True Image* appears.

→ Click on **Create Image**

2. The window *Create Image Wizard - Welcome to the Create Image Wizard* appears.

→ Click on **Next**

3. In the window *Create Image Wizard - Selecting Partitions to Image* select the partitions you want to image.

→ Click on **Next**

4. A window *Information* appears that informs about the possibility of an incremental image

→ Click on **OK**

5. The window *Create Image Wizard - Image Archive Creation* appears. Select the partition, drive or network drive where you want to store the image. The following steps describe archiving on a network drive

→ Click on **Next**

Please note that Acronis True Image is able to burn images to DVD with version 9.0 3.633 and higher. Previous versions can only store on CD, hard disks and network drives.

6. The window *Create Image Wizard - Creating Image Mode* appears. Select either a full backup or an incremental one. The following steps describe the creation of a full backup.

→ Click on **Next**

7. The window *Create Image Wizard - Image Archive Splitting* appears. It is recommended to choose *Fixed Size* and specify 650 MB. With this size you can afterwards burn the image files on CD if necessary.

→ Click on **Next**

8. The window *Create Image Wizard - Compression Level* appears, select *Maximum*.

→ Click on **Next**

9. The window *Create Image Wizard - Image Archive Protection* appears. You can enter a password to protect your image. If in doubt do not choose a password,

this makes it more save for the restoring of the image.

→ Click on **Next**

10. The window *Create Image Wizard - Image Archive Comments* appears. Enter important information about the current image. This makes it easy in the future to identify this image.

→ Click on **Next**

11. The window *Create Image Wizard - Imaging operation summary* appears. Check if everything is correct.

→ Click on **Proceed**

12. Creation of the image will start. This process will take about 20 minutes. When it is finished a window will appear with information *Image was successfully created.*

Chapter 16

File and directory handling

16.1 Viewing and opening files/directories

Windows XP offers three different ways of finding files or directories (folders). If you want to find a specific file and you have no idea where it resides, you can use the **Search** program. If you want to get an overview over the directory tree(s), you can use **Windows Explorer** or **My Computer**.

16.1.1 Windows Explorer

The Explorer provides an overview over all drives, directories and files in a two paned window.

1. Click **Start** → **All Programs** → **Accessories** → **Windows Explorer**

    or right-click **Start** → **Explore**

2. A double-paned window '*Exploring*' appears

    •   On the left side you see all drives and top level directories

    •   On the right side you see the contents of the drive or directory which is currently selected on the left side.

A drive or directory can be expanded in the left pane by clicking on the '+' button to the left of its icon. The '+' button changes to a '-' button. When you click the

icon itself, contents of the directory will appear in the right pane. A double-click on the icon, both expands the directory and shows its contents.
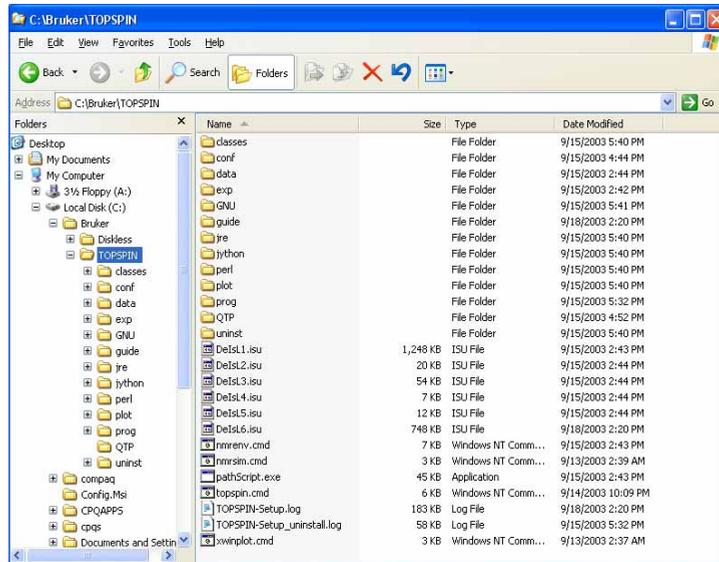
16.1.2 My Computer

The **My Computer** window provides an overview over all drives, directories and files. The differences under Windows XP between the **Explorer** and **My Computer** are very small. In fact you can use both windows with the same layout and handling.

1. Double-click the icon **My Computer** on the desktop

2. A window '*My Computer*' will appear, showing the computer's drives:

3. Double-click a drive, e.g. (C:)

4. A window showing the contents of the top level directory on C: will appear:

Double-click any icon. Depending on the file type, one of the following will happen:

- A directory (Folder) will be opened and its contents will be shown

- An executable program will be started

- A text file will be opened using an editor (by default **notepad**)

- For an unknown file type, a window '*Open with*' will appear, showing a list of available programs

If you click a directory icon two things might happen:

- the directory contents appears in a new window
- the directory contents replaces the contents of the current window

You can configure this feature according to your preference:

a) Double-click the icon **My Computer** on the desktop

b) Click **Tools → Options**

c) A window '*Options*' will appear:

- Click **General** and select one of the two **options** of '*Browse Folders*'

The disadvantages of a separate window for each directory is that your screen is soon filled up with windows. However, a quick way of closing an entire hierarchy of windows is the key combination **ALT+SHIFT+F4**.

If you want the explorer layout as a two paned window, select **View → Explorer Bar** and enable '**Folders**'. You are not able to store this configuration, this might be the biggest difference between the **Explorer** and **My Computer**

16.1.3 Explorer and My Computer can hide file extensions

Windows XP Explorer and My Computer allow you to hide known file extensions like `.txt`, `.fm`, `.doc` etc. One of the problems when you hide them is that the editor Notepad appends the extensions `.txt` to files which do not have a known extension. For example, `license.dat` is changed to `license.dat.txt` and thereby becomes unusable. Therefore, we recommend to configure My Computer such that it shows file extensions:

1. Double-click **My Computer**
2. Click **Tools → Folder Options → View**
3. Unselect **Hide file extensions for known file types**
4. Click **OK**

This setting also applies to Explorer.

16.1.4 Search

The Windows XP Find program allows you to search files and directories accord-

ing to various criteria.

Suppose you are looking for the file named `cosy`:

    a) Click **Start → Search → For Files or Folders**

       (or press **F3** when the cursor is on the desktop background)

    b) Click the small arrow right of the field **Look in**: select the drive on which you expect to find the file. If you select **My Computer**, all drives will be searched.

    c) In the field **Named**: enter `cosy`

    d) Click **Find now**

All files which contain the string `cosy` in their name will appear in the result, e.g. `cosy`, `cosygs`, `pecosy`. You can directly open the file by clicking on it. Furthermore, you can also search for text files which contain a certain string if you define it in the field '*Containing Text*'. Clicking on '**Search Options**' will show you some more parameters like '*Date*' or '*Size*' which you can added in your search options

16.1.5 The Windows Command Prompt

A Windows XP Command Prompt (shell) can be opened in three ways:

    • Click **Start → All Programs → Accessories → Command Prompt**

    • Click **Start → Run** enter **cmd** click **OK**

    • Press **CTRL+ESC → r** enter **cmd** click **OK**

A window will appear where you can enter Windows commands like **cd, dir, type, copy, ren, move, notepad, print, ipconfig, cacls, telnet, ftp** etc.

The default Prompt is **C:\>** when the computer was booted from this drive.

16.2 File and directory permissions

Windows XP supports file level security on NTFS but not on FAT filesystems. Note that TOPSPIN can only be installed on NTFS and as such it supports file level security.

16.2.1 Permissions and Types of Access

Folders and files can have the following permissions:

Permission	Full Control	Modify	Read & Execute	List Folder Contents[1]	Read	Write
Traverse Folder[1] / Execute File[2]	yes	yes	yes	yes	no	no
List Folders[1] / Read Data[2]	yes	yes	yes	yes	yes	no
Read Attributes	yes	yes	yes	yes	yes	no
Read Extended Attributes	yes	yes	yes	yes	yes	no
Create Files[1] / Write Data[2]	yes	yes	no	no	no	yes
Append Data	yes	yes	no	no	no	yes
Write Attributes	yes	yes	no	no	no	yes
Write Extended Attributes	yes	yes	no	no	no	yes
Delete Subfolders and Files	yes	no	no	no	no	no
Delete	yes	yes	no	no	no	no
Read Permissions	yes	yes	yes	yes	yes	yes
Change Permissions	yes	no	no	no	no	no
Take Ownership	yes	no	no	no	no	no
Synchronize	yes	yes	yes	yes	yes	yes

[1] folder permission

[2] file permissions

16.2.2 Changing file permissions

The permissions of a single file can be changed as follows:

1. Find the file in the Explorer (see chapter 16.1.1)

2. Right-click the file icon

3. Click **Properties**

4. A window '*Properties*' will appear:[1]

   • Click **Security**

5. Highlight the user/group for whom/that you want to change the permissions

6. Click **Allow** or **Deny** to set the permissions

7. If you want to add a new user/group click on **Add**

8. A window '*Select Users, Computers or Groups*' will appear:

   a) Select the one you are looking for **Add → OK**

9. Select the permissions you want to give to the new name

If you want to select special permissions, do step 1-5 then click **Advanced**

1. A window '*Access Control Settings for <filename>*' will appear:

   • Click **Permissions → View/Edit**

2. A window '*Permission Entry for <filename>*' will appear:

   • Click **Allow** or **Deny** of the permissions you want **OK → OK → OK**

16.2.3 Changing directory permissions

The permissions of a directory can be changed in the same way as file permissions:

In the window '*Permissions Entry for <directoryname>*' you can select in the Field '*Apply onto*' the effects of changing the permissions. Click the small arrow right of the field **Apply onto** and select the entry of your choice. You can select any combination between folder and/or subfolder and/or files **OK → OK → OK**

---

1. If Windows XP is installed the security section might be not displayed. If you like to see it, you have to define it in the options of Windows Explorer. Click on '**Tools**' → '**Folder Options**', click on '**View**' and disable the entry: '*Use simple file sharing (Recommended)*'

16.2.4 Read-only attribute

The problem of setting the **Read-only** attributes only in the entire directory and not in the subdirectory is solved under Windows XP:

1. Find the file or directory in the Explorer

2. Right-click its icon

3. Click **Properties**

4. A window '*Properties*' will appear:

   a)   Click the attribute **Read-only** to switch it on or off

5. A window '*Confirm Attribute Changes*' will appear where you are able to decide if your changes are set only for the entire directory or also for the subdirectories and folders.

16.3 Known Problems in TOPSPIN for Windows XP

AU programs which were copied from another computer are sometimes not displayed properly by Notepad. This happens if they were transferred with FTP in binary mode. You can either transfer the file again using **ftp** in ascii mode or with **rcp** or you can correct the local AU program as follows:

1. Start → All Programs → Bruker TOPSPIN → GNU Shell

2. vi au_program

   in the editor window enter:

   ```
   :set textmode
   :wq!
   ```

3. notepad au_program

   → the AU program should be displayed correctly now

16.4 Compressing files and directories

16.4.1 Setting the Compress attribute

For each file and directory under Windows XP, you can set so called attributes. One of these is the Compress attribute which reduces the size considerably.

1. Right-click a file or folder in the Explorer

2. A popup menu will appear:

   • Click **Properties**

3. A window '*<name> Properties*' will appear:

   a) Click **Advanced**

   b) Enable the attribute **Compress Contents to save disk space** → **OK** → **OK**

Compressed data will be uncompressed and recompressed automatically whenever they are accessed by an application. Note that this process will take time and your application runs slower when they work on compressed data. For transferring files or directories you might want to compress/archive them in zip format using the program Winzip rather than using the Compress attribute (see chapter 19.2).

16.5 Editing text files

You might know, UNIX doesn't write Carriage Returns (CR) at the end of text lines. That means that some files we create will not display properly in an editor like Notepad:

That doesn't mean that the file is damaged, it only means that the editor cannot resolve the issue. One reason to pick WordPad as an editor is that WordPad (unlike Notepad) is smart enough to render such files:
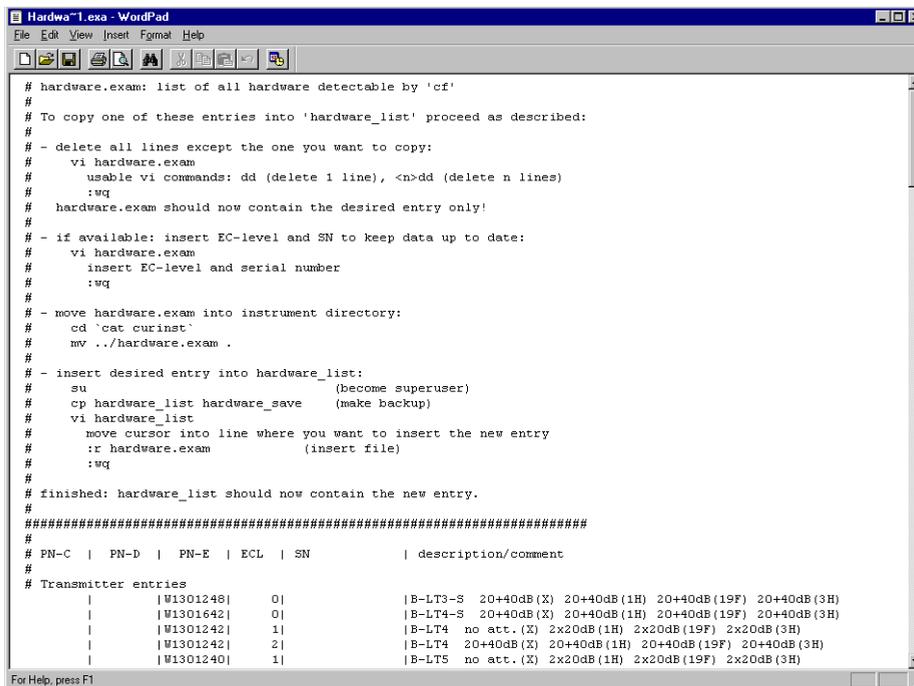
```
Hardwa~1.exa - WordPad                                                    _ □ ×
File  Edit  View  Insert  Format  Help

# hardware.exam: list of all hardware detectable by 'cf'
#
# To copy one of these entries into 'hardware_list' proceed as described:
#
# - delete all lines except the one you want to copy:
#     vi hardware.exam
#        usable vi commands: dd (delete 1 line), <n>dd (delete n lines)
#     :wq
#   hardware.exam should now contain the desired entry only!
#
# - if available: insert EC-level and SN to keep data up to date:
#     vi hardware.exam
#        insert EC-level and serial number
#     :wq
#
# - move hardware.exam into instrument directory:
#     cd `cat curinst`
#     mv ../hardware.exam .
#
# - insert desired entry into hardware_list:
#     su                           (become superuser)
#     cp hardware_list hardware_save    (make backup)
#     vi hardware_list
#       move cursor into line where you want to insert the new entry
#     :r hardware.exam             (insert file)
#     :wq
#
# finished: hardware_list should now contain the new entry.
#
###########################################################################
#
# PN-C  |  PN-D  |  PN-E  | ECL  | SN         | description/comment
#
# Transmitter entries
        |       |W1301248|      0|            |B-LT3-S  20+40dB(X) 20+40dB(1H) 20+40dB(19F) 20+40dB(3H)
        |       |W1301642|      0|            |B-LT4-S  20+40dB(X) 20+40dB(1H) 20+40dB(19F) 20+40dB(3H)
        |       |W1301242|      1|            |B-LT4  no att.(X) 2x20dB(1H) 2x20dB(19F) 2x20dB(3H)
        |       |W1301242|      2|            |B-LT4  20+40dB(X) 20+40dB(1H) 20+40dB(19F) 20+40dB(3H)
        |       |W1301240|      1|            |B-LT5  no att.(X) 2x20dB(1H) 2x20dB(19F) 2x20dB(3H)

For Help, press F1
```

Thus, if you see displays like the Notepad-example above, please try a smarter editor: WordPad comes with every Windows and those that have Microsoft Word can of course use Microsoft Word to edit files in luxury.

16.6 Upper/Lower case letters

The Windows file system NTFS intentionally does not differentiate between upper and lower case letters. Therefore working on a PC, please observe the following:

1. if you want to work with your SGI spectra on a PC avoid to create datasets with the same name differentiated only by being written in upper or lower case letters.

2. do not ignore the upper and lower case letters of TOPSPIN commands. If for instance you type **rpar PROT*** TOPSPIN will display the rpar-list of all parameter sets beginning with 'PROT'. The command **rpar Prot*** will show no parameter list, although the MS-Explorer displays the parameter set 'PROTON' in the wrong way 'Proton'.

Chapter 17

Plotting and Printing under Windows XP

17.1 Printing / plotting data

17.1.1 Plotting and printing

Under Windows XP, all common printer drivers are available and printers are installed with the Windows XP **add printer** tool (see chapter 14.1). When a printer is installed under Windows XP, it can be used for plotting from TOPSPIN and TOP-SPIN PLOT EDITOR.

The default printer and plotter for TOPSPIN are defined during the configuration of TOPSPIN by **expinstall** (see chapter 8.1.1).

17.1.2 Print/Plot from the Menu

The current data window can be printed as follows:

1. From the TOPSPIN menu:
    - Click the print button in the upper toolbar
    - or Click **File** → **Print**

- or Enter **`print`** or **`Crtl-p`**

All these actions are equivalent; they open the Print dialog box.
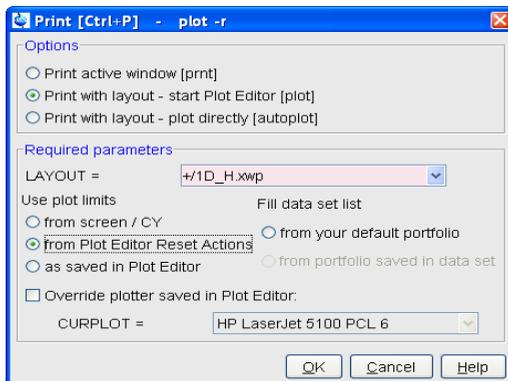
2. In the Print dialog box:

   a) Select ***Print active window [prnt]***

   b) Click ***OK***

   Before printing starts, the operating system print dialog box will appear to select e.g. the printer and printer properties.

   The Print dialog box contains two further options:

   - ***Print with layout - start Plot Editor [plot]***

     If you select this option and click OK, the Plot Editor will be started. This option is equivalent to entering plot on the TOPSPIN command line.

   - ***Print with layout - plot directly [autoplot]***

     Selecting this option activates the Plot Editor layout list box. Select the desired layout and click ***OK*** to print. Standard layouts are delivered with TOPSPIN. They use the Windows default printer. User defined layouts use the printer defined in the TOPSPIN PLOT EDITOR. On a 1D dataset, only 1D layouts are listed, on a 2D dataset only 2D layouts are listed etc.

   For the last two options, the following Required Parameters are available.

   Use plot limits:

   - ***from screen/ CY***

     The plot limits and maximum intensity are used as they are on the screen (processing parameter F1P, F2P and CY, respectively)

- *from Plot Editor Reset Actions*

    The plot limits and maximum intensity are set according to the TOPSPIN PLOT EDITOR Reset Actions (right-click inside the TOPSPIN PLOT EDITOR data field and choose Automation to set the Reset Actions).

- *as saved in Plot Editor*

    The plot limits and maximum intensity are set in the specified layout

Fill dataset list:

- *from your default portfolio*

    The portfolio contains the current TOPSPIN dataset plus the data from the default Plot Editor portfolio

- *from port folio saved in dataset*

    The portfolio contains the current TOPSPIN dataset plus the data from the portfolio stored in this dataset

17.1.3 Plot data from the Processing guide

Printing/plotting data can be done from the Processing guide by clicking the **Plot/Print** button. If **Automatic mode** is checked, the active data window will be printed as it appears in the screen. If **Automatic mode** is unchecked, you will get the dialog box.

17.1.4 Plot data with the TOPSPIN PLOT EDITOR

Although the **print** command allows you to use or start the TOPSPIN PLOT EDITOR, you can also start it from the command line (enter **plot**). This will open the TOPSPIN PLOT EDITOR from which you can create layouts and plot data. The complete TOPSPIN PLOT EDITOR functionality is described in its online manual that can be opened from the TOPSPIN PLOT EDITOR Help menu.

17.1.5 Print the Integral list

1. Click the Integrals tab of the data window

2. Enter **`print`**, *Ctrl+p* or right mouse click in the data window to print it

△ Object	Integral [abs]	Integral [rel]	Peaks	ν(F1) [ppm]	Intensity
⊟ Integral 1	216072656.66	1.0000	1		
└ Peak 1				3.8318	15.76
⊞ Integral 2	213030818.69	0.9859	1		
⊞ Integral 3	225346201.50	1.0429	1		
⊟ Integral 4	730954726.62	3.3829	3		
└ Peak 4				3.0861	17.34
└ Peak 5				3.0481	17.94
└ Peak 6				2.9600	18.94
⊞ Integral 5	325779960.75	1.5077	1		

17.1.6 Print the Peak list

1. Click the Peaks tab of the data window

2. Enter **`print,`** *Ctrl+p* or right mouse click in the data window

Peak	∨ ν(F1) [ppm]	Intensity	
1	3.8318	15.76	
2	3.3332	17.21	
3	3.1899	18.45	
4	3.0861	17.34	
5	3.0481	17.94	
6	2.9600	18.94	
7	2.6993	17.98	

17.1.7 Copy data to Other Applications

Under Windows XP, you can easily copy the data window contents to other applications. To do that:

- Click **Edit** → **Copy** [copy]

This will copy the data window contents to:

- the clipboard. After that you can paste the clipboard contents to any Windows application.
- the Windows Metafile file screenDump.wmf in the user properties directory (enter **`hist`** to locate this directory). The Windows Metafile can be imported by other applications or send to a different computer.

Note: Some programs, when importing spectra from the clipboard or metafile, do not display the contained information correctly. Particularly when you resize the

*imported graphics, sections of the text, the spectrum, or the axis sometimes have
disappeared.Usually this is only a display problem. When you print the respective
page, the representation is correct.*

17.1.8 Store (Export) a Data Window as Graphics File

The clipboard and metafile formats are resizable vector formats. In addition to this,
TOPSPIN allows you to save the contents of a data window in a graphics file of
selectable type, e.g. .png, .tif, .wmf etc. To do that:

1. Click **Edit → Export**
2. Navigate to the storage folder
3. Enter the destination filename and extension
4. Click *Export*

The resolution of such a screen dump equals the resolution of your screen. When
you import a graphics file into an other program, you may loose information when
resizing the graphics.

17.1.9 TOPSPIN PLOT EDITOR

1. TOPSPIN PLOT EDITOR uses the printer driver system of Windows XP for any
   printer output. This means that any printer for which a windows driver is cor-
   rectly installed can be selected as print device. Note that the printer name in a
   layout file written by the Windows XP version is probably not known by the
   UNIX version of TOPSPIN PLOT EDITOR because of the different printer han-
   dling. Apart from that, layout files can be freely interchanged between the two
   platforms.

2. TOPSPIN PLOT EDITOR uses the Windows XP Clipboard. If you put one or
   more TOPSPIN PLOT EDITOR objects to the clipboard then these are stored in
   windows metafile format. Therefore any windows application which is able to
   read metafile data from the clipboard can import TOPSPIN PLOT EDITOR
   objects.

3. Another way of exporting graphics is the menu option '*File/Export*' which
   allows you to save the complete layout in Windows Enhanced Metafile format
   (EMF). Most current graphical-oriented windows applications can import this
   format. This provides a convenient way of importing TOPSPIN PLOT EDITOR
   graphics into programs like Word or Powerpoint.

4. With the TOPSPIN PLOT EDITOR you can directly send your current plot as Email. Just click **File → Send** and TOPSPIN PLOT EDITOR will pop-up your default mail client and add the current plot as an EMF attachment.

Chapter 18

Windows XP commands

18.1 Important Windows XP functions and their shortcuts

The following Windows XP functions will be used regularly in this manual. They can all be started in different ways by mouse click or by entering a command on the keyboard. The following section describes some ways to start important functions:

1. Open the **Management Console**:
   - **My Computer** → right click **Manage**
2. Working as other User:
   - Right click on many icons → choose **Run as ...**
   - Right click in Explorer on many applications → choose **Run as ...**
   - Type in a command prompt:

     runas /user:administrator cmd.exe

     this will ask you for the administrator password and then open a Command prompt with administrator permissions
3. Open the Control Panel:
   - Click **Start** → **Control Panel**

- Click **My Computer** → **Control Panel**
- Press **Ctrl+Esc** → `s` → `c`

4. Open a Command Prompt:
   - Click **Start** → **All Programs** → **Accessories** → **Command Prompt**
   - Press **Ctrl+Esc** → `r` → enter `cmd` → click **Enter**

5. Open the Task Manager:
   - Click the RIGHT mouse button on the Taskbar → click **Task manager**
   - Press **Ctrl+Shift+Esc**

6. Search for files or directories:
   - Click **Start** → **Search** → **For Files or Folders**
   - Enter **Ctrl+Esc** → `s` → `s` → click **Enter**
   - Press **F3** while the focus is on the desktop
     (if the focus is not on the desktop: click on the desktop first)

7. Start the Windows Explorer:
   - Click **Start** → **All Programs** → **Accessories** → **Windows Explorer**
   - Right-click **Start** → **Explorer**
   - Double-click icon **My Computer** on the desktop

8. Configure the network:
   - Click **Start** → **Control Panel** → **Network Connections**
   - Right-click **My Network Places** → **Properties**

9. Close a hierarchy of windows opened from **My Computer**:
   - Press **Alt+Shift+F4**

More shortcuts may be found in chapter 18.3.1.

18.2 Online Help

Windows XP online help provides you with two kinds of help:

- help on specific topics
- help on what you see on your screen

18.2.1 Getting Help on specific topics

Click **Start** → **Help** (for a list of help topics)

- Click **Index** to get help on a predefined list of keywords
    - Enter the first letter(s) of a keyword
- Click **Find** to get help on all keywords contained in a data base

From the window which displays the help text you can go back to the main Help window by clicking **Help Topics**.

18.2.2 The question mark (?) in the upper right corner

Several windows, e.g. most windows which are opened from the Control Panel, have a question mark in the upper right corner. If you click it, the cursor will change to an arrow with a question mark. Now you can click a button or field you want information about. The information will disappear when you click the desktop background.

18.2.3 Tips on Windows XP

This window appears every time you log in, unless you unselect

Show this screen at startup

If you want this window back: click **Start** → **Run** enter `welcome` click **OK**

Click in the right window to read some tips.

18.2.4 Windows XP tips and tricks on the Web

Innumerous tips and tricks on Windows XP can be found on various Web pages.

18.3 Keyboard shortcuts

18.3.1 General Shortcuts

Function or mouse equivalent	Keyboard shortcut 1
Start	**CTRL+ESC**
Start → Documents	**CTRL+ESC d**
Start → Help	**- CTRL+ESC h** - **F1** from desktop or explorer
Start → Run	**- CTRL+ESC r** - **WIN+R**
Start → Search	**- CTRL+ESC c** - **F3** from desktop or explorer - **WIN+F**
Start → Shutdown	**CTRL+ESC u**
Taskbar → Task Manager	**CTRL+SHIFT+ESC**
Close the active window	**ALT+F4** [1]
Close a hierarchy of windows	**ALT+SHIFT+F4**
Switch to other task	**ALT+TAB**
Minimize all windows on desktop	**WIN+M**
Restore all windows as seen before	**WIN+SHIFT+M**
Toggle normal/full-screen Command Prompt	**ALT+ENTER**
Copy entire screen to Clipboard	**PRTSC** (Print Screen)
Copy active window to Clipboard	**ALT+PRTSC** (Print Screen)

1. Be careful: If no window is active Windows XP will prompt for reboot

18.3.2 Shortcuts for Windows Explorer

Function	Keyboard shortcut 1
Open new Explorer window	**WIN+E**
Rename file	**F1**
Open online help	**F2**
Open '*Find*' dialog	**F3**
Open '*Folder*' drop-down list	**F4**
Force refresh of windows contents	**F5**
Switch between left and right pane	**F6**
Go up one level in folder hierarchy	**BACKSPACE**
open context menu	**- SFHIFT+F10** - right mouse click

18.4 Command Prompt versus Graphical Interface

In a Windows environment, you normally work with a graphical interface, i.e. the **Start** button, Icons on the desktop, the Explorer etc. Nevertheless, Windows XP offers a Command Prompt, a shell, from which you can run various commands. The following table compares the Command Prompt with the graphical interface.

Function	Command Prompt	Graphical Interface
Files		
list files	**dir**	Explorer → Click **Drive** or **Folder**
delete a file	**del** (**erase**)	Right-click an icon in Explorer → **Delete**
rename a file	**ren**	Right-click an icon in Explorer → **Rename**
find text in files	**find**	**Start → Search → For Files and Folders → Containing text**

Function	Command Prompt	Graphical Interface
find a file		**Start → Search → For Files and Folders → Search for Files or Folders**
Directories		
make a dir.	**mkdir** (**md**)	**File → New → Folder**
remove a dir.	**rmdir**	Right-click icon in Explorer → **Delete**
change dir.	**cd <dir>**	Explorer
Utilities		
time and date	**date**, **time**	**Start → Settings → Control Panel → Date/Time**
backup	**ntbackup**	**Start → Programs → Accessories → System Tools → Backup**

18.5 Windows XP Command Prompt versus UNIX shell

Bruker BioSpin supports the TOPSPIN for both Linux and Windows XP. Here are some of the differences between these two operating systems which are of interest.

18.5.1 Directory specification

In a UNIX shell, pathnames are specified using the slash (/) character, whereas under Windows XP the backslash (\) character is used. Example:

UNIX shell: **cd /Bruker/TOPSPIN**

Windows XP Command Prompt: **cd \Bruker\TOPSPIN**

Under UNIX, command options are usually specified with a minus character (-) whereas in an Windows XP Command Prompt, the slash (/) character is used. For example, the command for listing files sorted by date:

UNIX shell: **ls -lrt**

Windows XP Command Prompt: **dir /od**

18.5.2 Windows XP commands versus UNIX commands

Under Windows XP, most commands can be executed via the Graphical Interface. You can, however, also open a Windows XP Command Prompt and run commands from there. Here is a list of UNIX shell commands and the corresponding Windows XP shell commands:

Function	UNIX shell	Windows XP Command Prompt
Files		
List files	`ls`	`dir`
copy a file	`cp`	`copy`
rename a file	`mv`	`ren`
delete a file	`rm`	`del` (`erase`)
print a file	`lp`	`print`
edit a file	`vi`, `jot`	`notepad`
display file contents	`cat`	`type`
sort a file	`sort`	`sort`
compare 2 files	`diff`	`comp`, `fc`
find text in file	`grep`	`find`
find a file	`find`	
Directories		
make a directory	`mkdir`	`mkdir`
remove a directory	`rmdir`	`rmdir`
copy a directory	`cp -r`	`xcopy`
change directory	`cd <dir>`	`cd <dir>`
show current directory	`pwd`	`cd`
Utilities		
time and date	`date`	`date`, `time`

Function	UNIX shell	Windows XP Command Prompt
manual pages	`man`	`help`
backup	`tar`	`backup` (`floppy`) or `ntbackup`(`tape`)

18.6 The UNIX GNU shell

For compatibility reasons, a UNIX shell is delivered on the TOPSPIN CD and automatically installed during the installation of TOPSPIN. When the installation is finished you can open a GNU shell by clicking:

Start → All Programs → Bruker TOPSPIN → GNU Shell

A GNU shell will open in which you can enter a restricted set of UNIX commands.

Chapter 19

Useful tools for Windows Windows XP

This chapter contains a description of some tools we found useful. We realize that many other tools are available for various purposes and we are very interested in your experiences. Just send your comments to:

> nmr-software-support@bruker-biospin.de

19.1 Update the operating system

There are two things that help you to be up-to-date with the operating system

- email notification about security fixes
- download and installation of hotfixes and service packs

Please see also chapter Microsoft Security Center (chapter 20.8).

Note: Bruker BioSpin recommends to choose the option 'Download updates for me, but let me choose when to install them' because the option 'Automatic download recommend updates for my computer and install them' could cause that the PC restarts automatically after the installation of an update.

19.1.1 Email notification about security fixes

Microsoft offers the possibility to subscribe for a newsletter that will inform you about security problems and their available fixes. Open Internet explorer and type in:

```
http://register.microsoft.com/regsys/pic.asp
```

You can subscribe there with your email address and after registration you can decide which kind of newsletter you want to get. It is recommended to subscribe at least for the *Microsoft Security Notification Service* to get all information about security leaks and their fixes.

19.1.2 Update of the operating system

- Click on **Start** → **All Programs** → **Internet Explorer Windows Update**

- The Internet Explorer will open. Click on **Tools** → **Windows Update**
  This will show a page where you can choose to start the search for all necessary updates.

- After the search is finished you have to choose which update of the available list you like to download.

- Start the download and follow the instructions.

19.2 Winzip: pack/unpack zip, tar, gz, uue files

The program Winzip allows you to pack or unpack archive files. The most common format is `.zip`, but Winzip also handles several other Windows and UNIX formats like `.tar`, `.gz` (created with gzip) and `.uue` (created with uuencode). An Evaluation Version of WinZip is available at: `www.winzip.com` which can be used for viewing and extracting archives. For creating archives, you should order an official version. Once Winzip is installed, it is automatically started when you click a file with the extension `.zip`, `.tar`, `.gz`, `.uue` etc. You can also drag and drop the file's icon into the Winzip window. Then click **Extract** to extract one file from the archive or click **Checkout** to extract all files.

19.3 Defragment your disk

Windows XP has an tool that allows you to defragment your disk. In the course of

time your disk will become more and more fragmented. Although an NTFS partition (which is required for TOPSPIN), suffers much less from fragmentation than a FAT partition, it might be a good idea to defragment it from time to time.

Start → All Programs → Accessories → System Tools → Disk Defragmenter

Chapter 20

Windows XP Tips and Tricks

20.1 Creating shortcut icons on the desktop

20.1.1 Creating shortcut icons to programs

For frequently used programs, it is convenient to create a shortcut icon on the desktop. For example, a shortcut to the editor **Notepad** can be created as follows:

1. Right-click the **Start** button
2. Click **Open**
3. A window '*Start Menu*' will appear:

   a) Click **All Programs** → Click **Accessories**
   b) Press and hold the right mouse button on the **Notepad** icon
   c) Drag the **Notepad** icon on the desktop, then release the right mouse button
   d) Click **Create Shortcut(s) Here**

Alternatively, you can click **Start** → **Search** to find the executable file Notepad.exe and perform step c to d. (see also chapter 20.1.2).

20.1.2 Creating shortcut icons to documents/files:

For frequently used files, it is convenient to create a shortcut icon on the desktop. If Windows XP recognizes the extension of the file, the corresponding program to read the file will be started, e.g. Word for a `.doc` file. For a text file without extension, you can specify the program to be used. e.g. notepad, in the shortcut properties. As an example we will use the TOPSPIN history file:

1. Find the directory `<var>\prog\curdir\<user>` in the Explorer

   e.g. `C:\Bruker\TOPSPIN\prog\curdir\guest`

2. Press and hold the right mouse button on the icon **history**

3. Drag the **history** icon on the desktop, then release the right mouse button

4. Click **Create Shortcut(s) Here**

   → an icon Shortcut to `history` will appear

5. Right-click the icon **Shortcut to history**

6. Click **Properties**

7. A window '*Shortcut to history properties*' will appear:

   a) Click **Shortcut**

   b) In the field **Target**: insert the program to be used before pathname, e.g.

      notepad C:\Bruker\TOPSPIN\prog\curdir\guest\history

   c) Click **OK**

20.2 Use the classic logon screen under Windows XP

To temporarily use the classic logon screen, press CTRL+ALT+DEL two times on the Welcome logon screen.

To configure Windows XP to use the classic logon and shutdown screens for every logon session, follow these steps:

1. Click Start, and then click Control Panel.

2. Double-click User Accounts.

3. Click Change the way users log on or off.
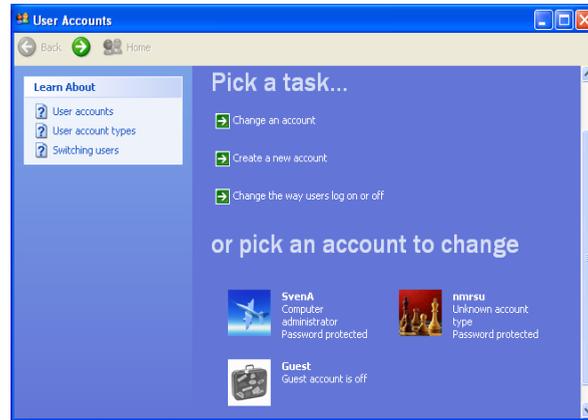
4. Clear the Use the Welcome screen check box.
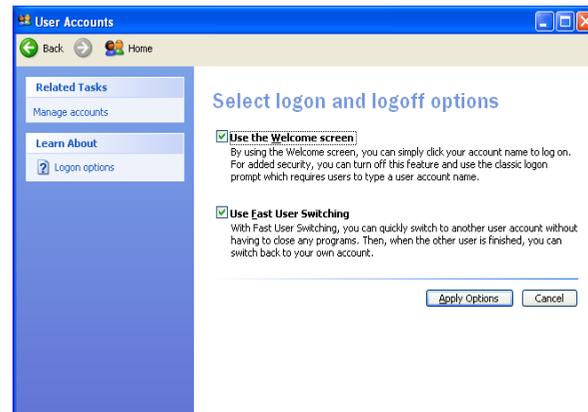
20.3 Convenient handling of TOPSPIN under Windows XP

20.3.1 Reading data from the Explorer into TOPSPIN

TOPSPIN can read data from the Explorer, via the Clipboard. Perform the following steps:

a) In the Explorer:
  • Find the dataset you want to display in TOPSPIN

- Right-click the data name folder
- A popup window will appear: click **Copy**

   b) In TOPSPIN:

- click *File → Paste*

You can also click a data expno or procno folder and read the corresponding dataset into TOPSPIN.

20.3.2 Copy a text item into the TOPSPIN command line

Any text item which can be copied to the Clipboard can be pasted to the TOPSPIN command line. Of course this is only useful if this text item is an existing TOPSPIN command. You can, for example, copy an TOPSPIN command from the manual to the command line:

1. Click *Help → Complete Processing Manual*

2. A PDF viewer (if installed) will start up showing the TOPSPIN processing manual:

   a) Click **Tools → Select text**
   b) Mark an TOPSPIN command in the manual, e.g. `search`
   c) Enter **Ctrl-C**

3. Move the cursor on the TOPSPIN command line:

4. Click the middle mouse button.

This feature is especially useful for long command names or commands with many arguments.The text can come form various sources, e.g. online documents, the Command Prompt, text editors. You can, however, not copy file or program names directly from the Explorer to the TOPSPIN command line.

20.4 Various useful configurations

This paragraph describes several settings that we found useful. They have no influence on the TOPSPIN performance and you are free to choose your own settings.

20.4.1 Configuring the Taskbar

1. Right-click the Taskbar [1]

2. Click **Properties**

3. A window '*Taskbar Properties*' will appear:

- De-select the item **Always on top**, click **OK**

This will create more space on the desktop.

20.4.2 Hide known file extensions

See chapter 16.1.3

1. Open the Explorer

2. Click the menu **Tools** → **Folder Options**

3. In the '*Folder Options*' window:

a) Select **VIEW**

b) Unselect **Hide file extensions for known file types** (if it is selected)

c) Click **OK**

20.4.3 Show hidden files and folders

1. Open the Explorer

2. Click the menu **View** → **Options**

3. In the '*Folder Options*' window:

a) Select **VIEW**

b) Select **Show hidden files and Folders**

c) Click **OK**

20.4.4 Configuring the GNU shell

The GNU shell is delivered on the CD '*TOPSPIN for Windows XP*' and is automatically installed together with the installation of TOPSPIN. It provides a set of UNIX commands. By default, the resize and cut & paste functions are not active.

Making the GNU window resizable by default:

1. Click **Start** → **All Programs** → **Bruker TOPSPIN** → **GNU Shell**

2. A GNU shell window will appear:

---

1. The taskbar is usually, but not necessarily, at the bottom of the screen

a) Click the symbol in the upper left corner of the window

b) Click **Properties**

3. A window '*GNU shell properties*' will appear:

a) Click **Layout**

b) In the field Screen Buffer Size:

- Set **Width** to 200
- Set **Height** to 100

c) Click **OK**

4. A window '*Apply properties to shortcut*' appears:

a) Click **Modify shortcut which started this window**

b) Click **OK**

Enabling the cut & paste function:

1. Click **Start → All Programs → Bruker TOPSPIN → GNU Shell**

2. A GNU shell window will appear:

a) Click the symbol in the upper left corner of the window

b) Click **Properties**

3. A window '*GNU shell properties*' will appear:

a) Click **Options**

b) Select **QuickEdit Mode**

4. A window '*Apply properties*' appears:

- Click **Apply properties to current window only**
- Click **OK**

The reason we do not recommend to enable the cut & paste function by default is that it would also count for the GNU shell started by TOPSPIN. Accidentally using cut & paste in that window could cause TOPSPIN to crash.

20.5 Connecting UNIX and Windows XP with Samba

Samba is a suite of programs which work together to allow clients to access UNIX file systems and printers via the SMB (Session Message Block) protocol.

In practice, this means that you can 'share' disks and printers with UNIX systems. You can then access them from LanManager clients, Windows for Workgroups 3.11 clients, Windows95 clients, Windows NT clients, Windows 2000 clients, Windows XP clients and OS/2 clients. A 'share' is a term used to describe resources (directories, printers, etc.) that the server is making available for others on the network to use.

More information you may find in chapter 13.4.3, in the directory `/usr/samba/README` and `/usr/samba/docs` or if you have Internet access on http://samba.org

The license conditions are described in `/usr/samba/COPYING`.

20.5.1 Accessing the network share provided by Samba

5. You can access shares from any Windows XP PC using the **Run**… feature available from the **Start** button.
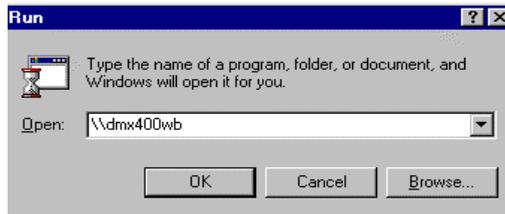
Type in two back-slashes followed by the (UNIX-)computer name (this operation is equivalent to running a '`find`' on a particular computer.

6. The corresponding response shows up in a Windows Explorer window:

You can double-click on the share you want to see and it will come up with either a

password request for shares with managed access…

… or the list of contents (in yet another Explorer window):
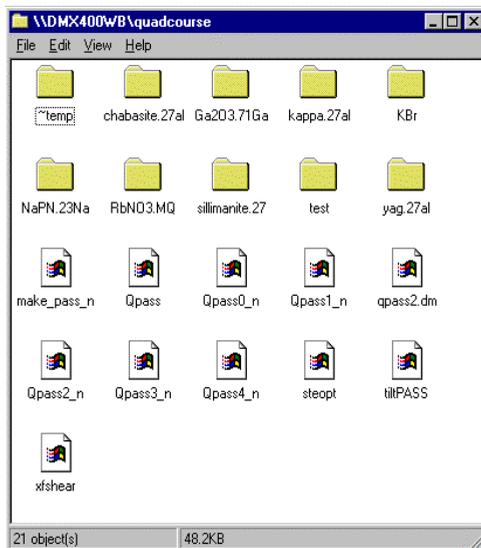
If you cannot get access to a share that you see and you are confident that the password is correct please see chapters 20.5.3 and 20.5.4.

To copy files you can drag-and-drop them from a content display and deal with files and directories as if they where local (e.g. you can drag-and-drop acqu-files into a Wordpad-icon on you desktop. Technically the job of making a connection is completed here.

20.5.2 Mapping network shares into 'local' drives

For some applications (including TOPSPIN) you will need, however, to map the network share to a (virtual) disk drive. That is: You create a look-alike of a local drive like, say, U: that points to the share you assign to it. Doing this is very simple:

Step #1: click with the right mouse button on the share you want to map to a disk drive

Select '**Map Network Drive**' (as shown).

Step #2: Select an appropriate drive letter (here: U:) and decide whether or not to click the '**reconnect at logon**' box. If you want a permanent connection that automatically is re-established any time the (client) PC is booting up click this box. If you don't check it this connection will only last until the next reboot.
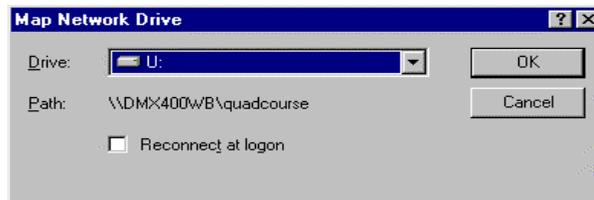
Step #3: Press '**OK**'. As you press '**OK**' the system will connect this network share as a new drive called U: You can look up the new virtual disk in Windows Explorer after a few seconds:
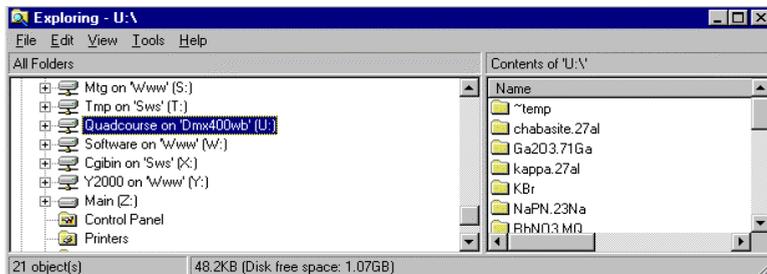
On the right-hand side the files shared out from UNIX are shown and you can go about copying, moving etc just like with native Windows files.

20.5.3 *Configuring Windows XP to handle UNIX-style password requests*

One of the most annoying problems with SAMBA is that older versions are not able to authenticate network connectors using encrypted passwords. In SAMBA 2.0.x the default setting is still plain password but you could change it to encrypted. T2.1his is the best way for the security of your network. If you want to use the plain-text password, it is possible on Windows XP side, to enable the authentication with clear-text passwords sent over the networking enabling the respective registry key (see the following chapters 20.5.5 and 20.5.4)

Note: THIS INTRODUCES A SIGNIFICANT SECURITY LEAK!

20.5.4 Enable Plain Text Password

1. Log in as administrator.

2. Click **Start → Control Panel**

3. Click **Administrative Tools → Local Security Policy**

4. Enable the tree **Local Policies → Security Options**

5. On the right side double click the entry '**Send unencrypted password to ...**'

6. Click on '**enabled**'

7. If your computer is part of a Windows NT / 2000 / XP domain contact your domain administrator about this policy setting and its interaction with possible 'group policies'

20.5.5 There is one shortcut you can try with newer samba-versions

They deliver a file called `WinXP_PlainPassword.reg` in the `../samba/docs` directory. If you can locate this file in the Windows Explorer and double-click it, it will automatically make the additions to the registry file detailed hereafter. If you double-clicked the file and it worked you are done here. If not, you need to proceed as detailed in chapter 20.5.4 and manually make the necessary changes.

20.6 How to log on to Windows XP if you forget your password

20.6.1 Method 1: Log On as an Administrator and Reset the Password

If you can not log on to Windows by using a particular user account (including the Administrator or Computer Administrator accounts), but you can log on to another account with administrative privileges (including the Administrator or Computer Administrator accounts), follow these steps:

1. Log on to Windows by using the administrator account that has a password that you remember.

   Note: You cannot log on as usual by using the Administrator or Computer Administrator account to a Windows XP Professional-based computer in a workgroup. To log on as the Administrator or Computer Administrator, you must start Windows XP in Safe Mode.

2. Click **Start** → Click **Run**.

3. In the Open box, type the following command, and then click **OK**:

   `control userpasswords2`

4. Click the user account that you forgot the password for → Click **Reset Password**.

5. Type a new password in both the New password and the confirm new password boxes → Click **OK**.

You should now be able to log on to Windows with the user account and the new password.

WARNING: If you reset the password for a user account in this manner in Windows XP Professional, the following types of information for that user will be no longer available:

   • E-mail messages that are encrypted with the user's public key

   • Internet passwords that are saved on, or remembered by, the computer

   • Any files that the user has encrypted

20.6.2 Method 2: Use a Password Reset Disk

If you created a password reset disk for Windows XP, you are able to reset your password by using the password reset disk. For additional information about how

to use a password reset disk, please check the articles in the Microsoft Knowledge Base:

- In order to create and use a Password Reset Disk for a computer that is not a domain member in Windows XP please read:

  ```
  http://support.microsoft.com/default.aspx?scid=kb;EN-
  US;305478
  ```

- In order to create and use a Password Reset Disk for a computer in a domain in Windows XP please read:

  ```
  http://support.microsoft.com/default.aspx?scid=kb;EN-
  US;306214
  ```

20.7 Error Message When You Use the Add Printer Wizard

When you create a printer (either a local printer or a remote network printer) by using the *Add Printer Wizard*, you may receive the following error message: "Operation could not be completed. The print spooler service is not running."

This error occurs because the Spooler service has not been started or has stopped working. To start the Spooler service, follow these steps:

1. Click **Start** → Click **Control Panel**.
2. Double-click **Administrative Tools** → Click **Services**.
3. Double-click the **Printer Spooler** service → Change the startup type to **Automatic**. This sets the Spooler service to start automatically when you restart the computer.
4. If you want to start the spooler service immediately, click the **Start** button under the **Service Status** field.

20.8 Microsoft Security Center

If you connect your computer to the Internet, you can be vulnerable to viruses, worms, hackers, and other Internet intruders. To help protect your computer against viruses and other security threats, Bruker BioSpin recommends to have a firewall and updated antivirus software running at all times.

Microsoft Windows XP Service Pack 2 (SP 2) contains the new Security Center, which helps you to manage your computer's security settings and therefore more

secure. If you are not running a firewall or an up-to-date version of antivirus software, you will see an alert in the notification area, to the right of the taskbar.

Wit the help of the Security Center you can check the status of the important security settings. You can also use it to find information about the latest virus or other security threat or to get customer support from Microsoft for a security-related issue.

20.8.1 How to open Security Center

1. Click **Start** → **Control Panel**.
2. Double-click **Security Center**. A window 'Microsoft Security Center' will appear:

The Security Center helps to check that you have:

- A software firewall.
- Configure the settings for Automatic Updates.
- An up-to-date antivirus program.

If the Security Center detects that your computer might benefit from enhanced security in one of the three areas (Firewall, Automatic Updates and Antivirus program), it displays an alert in the notification area (to the right of the taskbar). An

alert message is displayed every time you log on, until the problem is fixed.

Windows Security Center checks for many common antivirus and firewall programs, but it is possible that you might be using a program that Windows can't find. If you are not sure about the status of your antivirus or firewall solution, or if you receive a Security Center alert that seems incorrect, check with your antivirus or firewall vendor to find out if the software you are running is supported in the Security Center.

Note: If your computer is part of a domain, your security settings are typically managed by your network administrator. In this case, the Security Center does not display your security status or send alerts.

20.8.1.1 What do the new security icons mean?

Windows XP SP2 contains a set of security icons that can help you recognize potential security risks and choose appropriate security settings.

These icons means:

-    Indicates important security information and settings.

-   Notifies you of a potential security risk.

-   Situation is more secure. Your computer is using recommended security settings.

-   Warning: situation is potentially harmful. Consider adjusting security settings to enhance the security of your computer.

-   Your computer's current security settings are not recommended.

20.8.2 Firewall

Windows Firewall, previously known as Internet Connection Firewall or ICF, is a protective tool that monitors and restricts information that travels between your computer and a network or the Internet. This provides a line of defence against someone who might try to access your computer from outside the Windows Firewall without your permission.

Bruker BioSpin recommends to protect your computer against viruses or security threats, we recommend to keep the Windows Firewall (or another firewall) on.

20.8.2.1 To open Windows Firewall

1. Click **Start** → **Control Panel**.
2. In the window **Control Panel** → click **Windows Security Center**.
3. Click **Windows Firewall**.
4. A window 'Windows Firewall' appears:
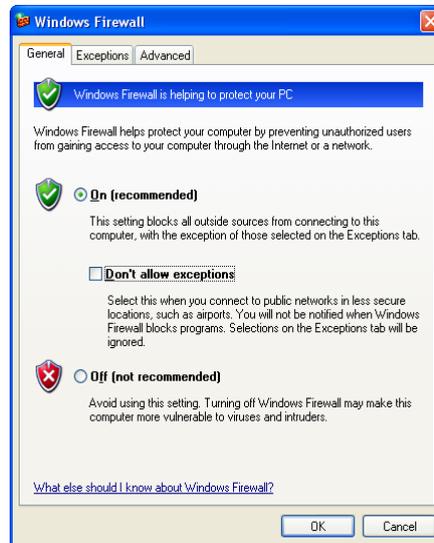
Because a firewall restricts communication between your computer and the Internet, you might need to adjust settings for some programs that prefer an open connection. These adjustments are called 'exceptions'.

Windows Firewall now has three settings:

1. **On:** Windows Firewall is turned on by default, and normally you should leave it that way. When you choose this setting, Windows Firewall blocks all unsolicited requests to connect to your computer, except for requests to programs or services selected on the **Exceptions** tab.

2. **On with 'Don't allow exceptions':** When you select the **Don't allow exceptions** check box, Windows Firewall blocks all unsolicited requests to connect to your computer, including requests to programs or services selected on the

Exceptions tab. Use this setting when you need maximum protection for your computer (e.g. when you connect to a public network in a hotel or airport)

There is no need to keep **Don't allow exceptions** selected all the time, because when it is, some of your programs might not work correctly, and the following services are blocked from accepting unsolicited requests:

- File and Printer Sharing
- Remote Assistance and Remote Desktop
- Discovery of network devices
- Preconfigured programs and services on the exceptions list
- Additional items that you've added to the exceptions list

3. **Off:** This setting turns Windows Firewall off. When you choose this setting, your computer is much more vulnerable to harm from unknown intruders or viruses. This setting should only be used by advanced users for computer administration purposes, or if your computer is protected by another firewall.

20.8.2.2 Windows Firewall settings

If you are running Windows XP SP2 the Windows Firewall is turned on by default. This means that most programs will not be allowed to accept unsolicited communications from the Internet unless you choose to list those programs as exceptions. There are two programs that, by default, are already added to the exceptions list: **Files and Settings Transfer Wizard** and **File and Printer Sharing**.

Because firewalls restrict communication between your computer and the Internet, you might need to adjust settings for some other programs that prefer an open connection. You can make an exception for these programs, so that they can communicate through the Windows Firewall.

Each time you allow an exception for a program to communicate through Windows Firewall, your computer is made more vulnerable. If you have lots of exceptions and open ports, your computer can become more vulnerable. To help decrease your security risk:

- Only allow an exception when you really need it.
- Never allow an exception for a program that you don't recognize.
- Remove an exception when you no longer need it.

Sometimes you might want someone to be able to connect to your computer,

despite the risk such as when you expect to receive a file sent through an instant messaging program.

You can use the Bruker BioSpin `setfirewall.cmd` script to configure the Windows firewall (see chapter 8.9).

Note: The firewall for the spect ethernet card has to be disabled!

20.8.2.3 To add a program to the exceptions list

1. Click **Start** → **Control Panel**.
2. In the window **Control Panel** → click **Windows Security Center**.
3. Click **Windows Firewall**.
4. A window 'Windows Firewall' appears:.
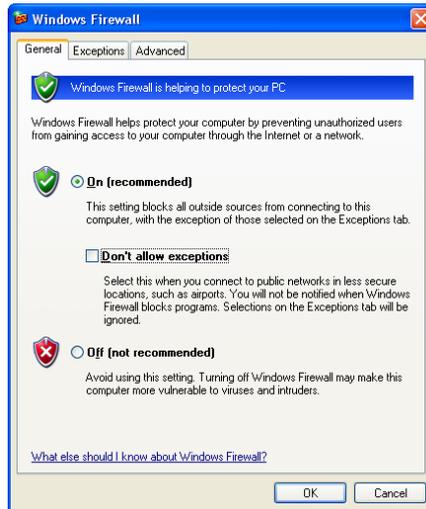
5. Click on the **Exceptions** tab. Under **Programs and Services**, select the check

box for the program or service that you want to allow, and then click **OK**.
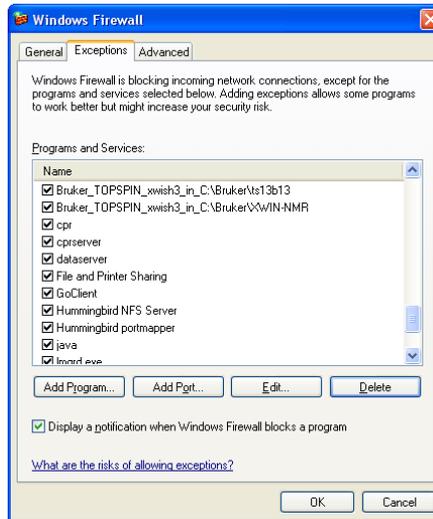
20.8.2.4 Add a program (or service) to the exception list

1. Click **Start → Control Panel**.

2. In the window **Control Panel →** click **Windows Security Center**.

3. Click **Windows Firewall**. A window appears → click on the **Exceptions** tab.
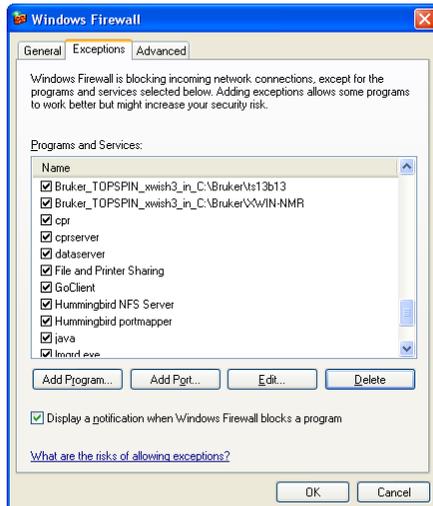
4. Click on **Add a Program**. This will open a dialog box.
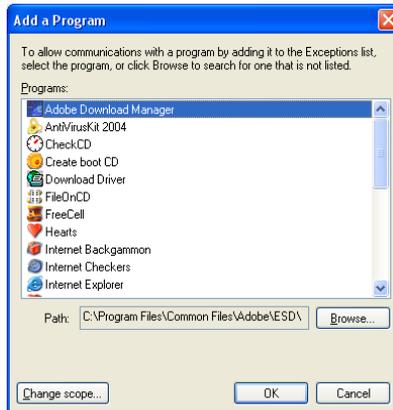
Click the program that you want to add, and then click **OK**. The program will appear, selected, on the **Exceptions** tab, under **Programs and Services**.

5. Click **OK**.

20.8.2.5 Open a Port in the exception tab

If you still do not find the program, you can open a port instead (When you open a port, remember to close it again when you are done using it.).

Adding an exception is preferable to opening a port because it is more secure than opening a port, because the firewall is only open while the program is waiting to receive the connection.

1. Click **Start** → **Control Panel**.

2. In the window **Control Panel** → click **Windows Security Center**.

3. Click **Windows Firewall**.

4. A window 'Windows Firewall' appears. Click on the **Exceptions** tab.
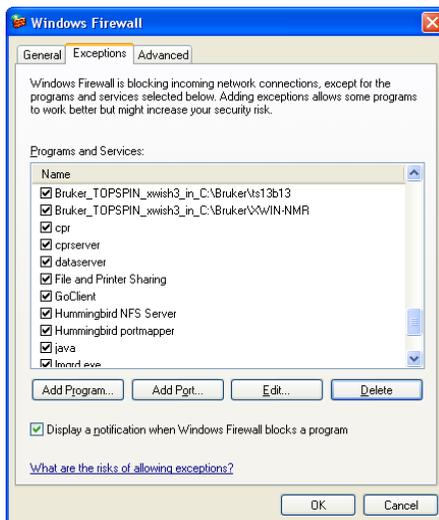
5. Click on **Add a Port**. This will open a dialog box.

Click the program that you want to add → click **OK** → click **OK**.

20.8.2.6 Advanced Options

Advanced users can open ports for, and configure the scope of, individual connections to minimize opportunities for intruders to connect to a computer or network. To do this, open the Windows Firewall, select the Advanced tab and use the settings under Network Connection Settings.

1. Click **Start** → **Control Panel**.

2. In the window **Control Panel** → click **Windows Security Center**.

3. Click **Windows Firewall**.

4. A window 'Windows Firewall' appears. Click on the **Advanced** tab.
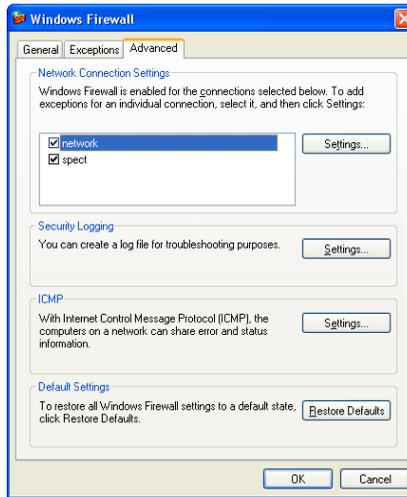
5. Click under Network Connection Settings on Settings.
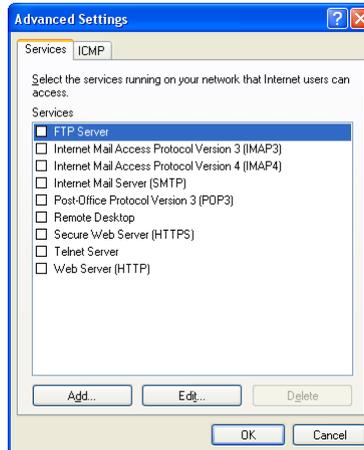
6. Click **OK**.

20.8.2.7 How to disable Firewall Alerts from the Security Center

If you have installed another firewall than Windows Firewall, the Security Center may still be able to tell you the status of that firewall and may also display an alert if it stops working.

There are some firewalls that Windows Security Center will not find, such as a

hardware firewall or certain types of software firewalls. If your computer is using a hardware firewall, you should not disable Windows Firewall. If you install and run another firewall, you should turn off Windows Firewall. If you use another software firewall that Windows doesn't recognize, you may want to disable the Security Center firewall alerts.

Note: You should only disable these alerts if you are sure that your computer is protected by a firewall. The following procedure assumes that you have already turned off Windows Firewall and that you have received an alert telling you that you do not have a firewall installed.

20.8.2.8 How to specify a firewall that Windows does not find

1. Click **Start** → **Control Panel**.
2. Double-click **Security Center**.
3. Select **Firewall** → click **Recommendations**. (*Note: The Recommendations button is not available when your Firewall setting is marked **ON**.*)
4. In the **Recommendations** dialog box, select the '**I have a firewall solution that I'll monitor myself'** check box → click **OK**.

When you use this procedure, the Security Center displays your Firewall setting as Unknown, and does not send you alerts.

20.8.3 Automatic Updates

Windows Security Center allows you to easily manage security settings for Automatic Updates. When you turn on Automatic Updates, Windows routinely checks the Windows Update Web site for high-priority updates that can help protect your computer against attacks. High-priority updates include security updates, critical updates, and service packs.

20.8.3.1 How to change your Automatic Updates settings

By default, any new updates are installed each day at 3 a.m.

1. Click **Start** → **Control Panel**.
2. Double-click **Security Center**.
3. Under **Manage your security settings for** → click **Automatic Updates**

4. A window 'Automatic Update' will appear:.
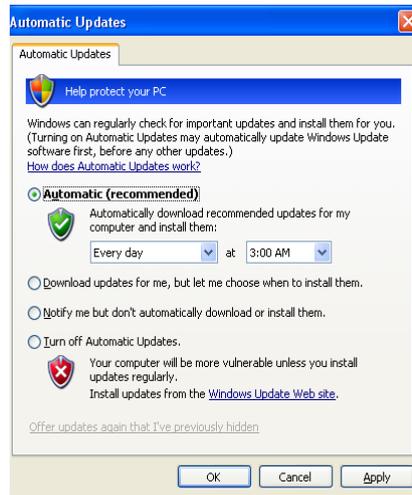
The options for Automatic updates are:

- Automatic: Automatic download recommend updates for my computer and install them: e.g. 'Every day' at '3:00 AM'

- Automatic: Download updates for me, but let me choose when to install them (recommended by Bruker BioSpin for PCs which controls spectrometer.
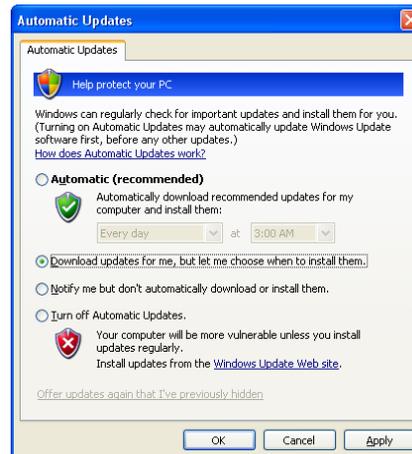
- The Updates are downloaded behind the scenes whenever you are connected to the Internet. The downloading process does not interfere with other

downloads or interrupt you while you work. If you disconnect from the Internet before updates are fully downloaded, the download process will continue the next time you connect to the Internet.

- Automatic: Notify me but do not automatically download or install them.
- Turn off Automatic Updates. Your computer will be more vulnerable unless you install updates regularly. Install updates from the Windows Update Web site.

You can also visit the Windows Update Web site on a regular basis to get updates for your computer. The Web site provides the same high priority updates as Automatic Updates, but also offers optional updates that can help improve your computer's performance or add functionality to some of your programs.

Bruker BioSpin recommends to choose the option 'Download updates for me, but let me choose when to install them' because the option 'Automatic download recommend updates for my computer and install them' could cause that the PC restarts automatically after the installation of an update.

20.8.4 Antivirus

20.8.4.1 How to disable Antivirus Alertsform the Security Center

If you are running Windows XP SP2 Windows Security Center should tell you about the status of your antivirus software and display an alert if it stops working. Some antivirus programs are designed to report specific information about the program to the Security Center.

However, not all antivirus programs are designed to report to the Windows Security Center. In fact, there are some antivirus solutions that the Security Center will not detect at all. If you use an antivirus program that Windows does not recognize, and you keep it up to date and properly configured, you may want to disable the antivirus Security Center alerts.

Note: You should only disable these alerts if you are sure that your computer is protected by the full version of an up-to-date antivirus program. In addition, once you disable alerts, even if your program receives an update that makes it fully detected within Security Center, you will not receive alerts unless you clear this check box.

20.8.4.2 How to specify an antivirus program that Windows does not find

1. Click **Start → Control Panel**.

2. Double-click **Security Center**.

3. In the Security Center, under **Virus Protection**, click **Recommendations**. (The Recommendations button is not available when your Virus Protection setting is marked ON.)

4. In the **Recommendations** dialog box, select the **I have antivirus software that I'll monitor myself** check box, and then click **OK**.

When you use this procedure, the Security Center displays your Virus Protection setting as Unknown, and does not send you alerts.

20.8.5 Microsoft Pop-up Blocker

With the Windows XP SP2 Internet Explorer you are able to prevent most pop-up windows from appearing over Internet pages you want to view while you are using the Internet.

Many advertisers on the Internet use windows that pop up in the middle of your screen to display a message. They might also open when you click a link or button on a Web site, and they might open either over or under the window you wish to view. Some pop-ups are helpful. Unfortunately, some pop-up windows can contain inappropriate content or can be a way for you to accidentally download dangerous software (called spyware or adware) onto your computer.

When you install SP2, Pop-up Blocker is turned on in Internet Explorer and set to the medium setting, which means it will block most automatic pop-ups. The default settings for the pop-up blocker allow you to see pop-ups that are opened when you click a link or button on a Web site. Pop-up Blocker will also play a sound and show the Information Bar when a Pop-up is blocked. You can adjust these settings so that Pop-up Blocker works the way you want it to.

20.8.5.1 How to change Pop-up Blocker settings

1. Open the Microsoft Internet Explorer.

2. On the **Tools** menu, select **Pop-up Blocker** → click **Pop-up Blocker Settings**.
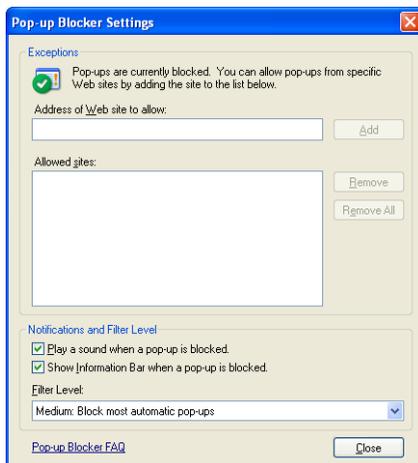
If you want to see pop-up windows from a specific Web site, type the address (or URL) of the site in the **Address of Web site to allow** box, and then click **Add**.

If you would like to temporarily allow a site to display pop-ups, click the Information Bar when it notifies you that a pop-up has been blocked → click **Temporarily Allow Pop-ups.**

20.8.5.2 How to block pop-ups when you click a link (or button) on a Web site

1. Open Internet Explorer.

2. On the **Tools** menu, select **Pop-up Blocker** → click **Pop-up Blocker Settings**.

3. Select the **High** setting in the box near the bottom of the dialog box.

Note: If you want to see pop-ups that are blocked when you have this setting turned on, hold down the CTRL key while the window opens.

20.8.5.3 To turn on Pop-up Blocker

1. On the **Tools** menu, select **Pop-up Blocker**.

2. Click Turn on Pop-up Blocker.

If you get similar pop-up windows no matter what sites you visit or even if you are not on the Web at all, you could have spyware, adware, or other software on your computer that's launching pop-ups. To stop these pop-ups, you will have to iden-

tify the software, then remove it or change its settings to stop it from launching pop-ups.

Pop-up Blocker will not block pop-up windows that you open deliberately by clicking a link. For example, if you were on a travel reservation site and you clicked a link to open a pop-up window containing your confirmation details, this pop-up window would not be blocked because you opened it intentionally. The Pop-up Blocker will not block some pop-ups with certain types of animated content or pop-ups from Web sites that are in two Web content zones: *Local intranet* or *Trusted sites*.

20.8.6 Multilingual User Interface Pack (MUI) for Microsoft Windows XP Professional

The *Multilingual User Interface Pack* (MUI) is a special package with a set of language specific resource files which can only be added to the English version of Windows XP Professional. The *Multilingual User Interface Pack* allows (when installed) the user interface language of the operating system to be changed according to the preferences of individual users to one of the supported (and installed) languages. Local users can then select the user interface language or it can be set by group policy for organizational units.

The *Multilingual User Interface Pack* also allows different language users to share the same workstation. For instance, one user might choose to see system menus, dialogues and other text in German, while another user logging onto the same system might prefer to see the corresponding text in Hungarian.

On Windows PCs delivered by Bruker BioSpin the 'Multilingual User Interface Pack' for Microsoft Windows XP Professional is preloaded. The following languages are available: English (default), Chinese (Simplified), Chinese (Traditional), Finnish, French, German, Hungarian, Italian, Japanese, Korean, Polish, Spanish, Swedish, Turkish

Note: Multilingual User Interface Resource Files are only sold as a bundle with the English version of Windows. It is not available through retail channels.

For further information please refer to:

```
http://www.microsoft.com/globaldev/DrIntl/faqs/muifaq.mspx#MUIques1
```

20.8.6.1 Change the user interface language

The appropriate Menus and dialogues language can be selected from the Regional Options applet in Control Panel.

1. Click **Start → Control Panel**.

2. Double-click **Regional and Language Options**.

3. Click on the **Languages** tab.
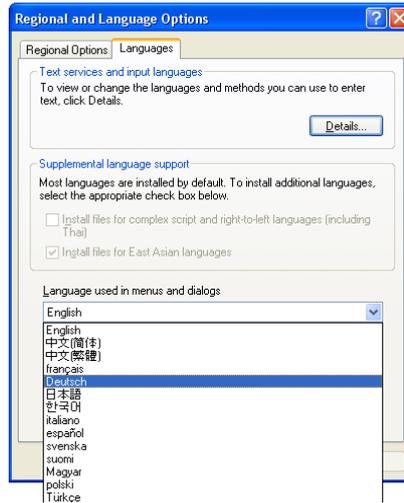
The Menus and dialogs drop down list will display all the installed languages.

Note: Changes to the user interface language only become effective after logging off and logging on again.

For further information please see:

```
http://www.microsoft.com/globaldev/refer-
ence/win2k/setup/changeui.mspx
```

Chapter 21

Appendix

21.1 Some notes for the helium handling

In the TOPSPIN installation path (normally `C:\Bruker\TOPSPIN`) in the directory `...\prog\logfiles` are two files named `heliumlog` and `heliumlog.err`. The `heliumlog` saves every night at 3.00 am the actual helium level in a new line. The `heliumlog.err` documents every error during detecting the helium level.

The helium log runs under the local system account. Change this to the user whois always logged on:

  a) Click on **Start → Settings → Control Panel →** 'Task Scheduler'.
  b) Click twotimes on the task AT1(2,...) which runs at 3:00 AM.

21.1.1 Automatic notification for helium refill

1. Open a Command Prompt and enter:

  • **cd /d c:\Bruker\TOPSPIN**
  • **notepad heliumlimit**

type in the number (without '%') of the helium level should activate the notification, e. g. **25**

Click **file** → **save as ..** and save it as **`<TOPSPINHOME>\heliumlimit`**

Of course, you can also install the heliumlimit file from the Explorer. We have chosen the Command Prompt because the Explorer might add the extension `.txt` to the file `heliumlevel` which makes it unusable (see chapter 7.2.2).

2. Now you could create a command script <TOPSPINHOME>\heli-umwarn.cmd that will be executed if the actual helium level is the same or below the entry (in %) in the file <TOPSPINHOME>\heliumlimit

E. g. it is possible to create a message window on the screen of the spectrometer PC and/or every other PC in your network (e. g. the PC of the responsible person for helium refill). You could do this in the following way:

3. Open a Command Prompt and enter:

- **`cd /d c:\Bruker\TOPSPIN`**

- **`notepad heliumwarn.cmd`**

type in the following text:

```
@echo off
rem -------------------------------------------------------
rem heliumwarn.cmd: example MS cmd script to send a warning
rem                 argument1=LEVEL
rem                 argument2=LIMIT
rem -------------------------------------------------------
rem  user defined variables:
rem  INSTRUMENT: is the name of the spectrometer
rem  ADDRESS   : the address where the message is sent to.
rem              type 'net help send' for details
rem -------------------------------------------------------
set INSTRUMENT='Avance-300'
set ADDRESS1=%COMPUTERNAME%
set ADDRESS2=%NMR-SUPERUSER-PC%
set ADDRESS3=%HELIUM-REFILLER-PC%
rem ----------------------------
rem  catch command line arguments:
rem ----------------------------
set MYSELF=%0
```

```
set LEVEL=%1
set LIMIT=%2
rem ---------------------------------------
rem  get the name of the spectrometer host:
rem ---------------------------------------
set HOST=%COMPUTERNAME%
rem ---------------------------
rem  prepare the email message:
rem ---------------------------
set MSG=Attention: At the magnet of the %INSTRUMENT% spec-
trometer is the heliumlevel of %LEVEL%%% equal or lower than
the helium level limit of %LIMIT%%%: please order liquid he-
lium and refill the helium tank. --- This message has been
sent by %MYSELF% on %HOST% to %ADDRESS1%, %ADDRESS2% and
%ADDRESS3%
rem ------------------
rem  send the message:
rem ------------------
net send %ADDRESS1% %MSG%
net send %ADDRESS2% %MSG%
net send %ADDRESS3% %MSG%
```

You have to write in your individual parameters

- replace Avance-300 with the name of your spectrometer
- replace NMR-SUPERUSER-PC with the name of the PC of the NMR-Supe-ruser
- replace HELIUM-REFILLER-PC with the name of the PC of the responsible person for helium refill
- Attention - the text sequence:

  set MSG=Attention: At the magnet of the %INSTRUMENT% spectrometer is the heliumlevel of %LEVEL%%% equal or lower than the helium level limit of %LIMIT%%%: please order liquid helium and refill the helium tank. --- This message has been sent by %MYSELF% on %HOST% to %ADDRESS1%, %ADDRESS2% and %ADDRESS3%

had to be written in one line!

click **file** → **save as..** and save it as **`<TOPSPINHOME>\heliumwarn.cmd`**

Now the defined PC's will get an error message if the actual helium level is the same or below the entry (in %) in the file

`<TOPSPINHOME>\heliumlimit`

The notifications were sends only once but it will be activated again if the helium level is against higher than the limit.

Note that this script is only an example, if you would like to add more PC's in the notification list you had to add the respective addresses, if you like to have-less addresses you have to delete the respective entries.

21.2 Script for saving important files

TOPSPIN offers a script (xwinnmr.save) for saving very important files that are not delivered by BRUKER. This script can save and extract user specific data from the TOPSPINHOME directory and puts them into a tar-file. Files that start with an "." are ignored. The script can be started as follows:

• Click on the Bruker Utilities icon on the desktop

   Bruker Utilities → *Miscellaneous* → *xwinnmr.save.cmd*

• For more information open the command prompt of the Bruker Utilities

   Bruker Utilities → *Command prompt*   and enter

   `.\prog\bin\utilities\miscellaneous\xwinnmr.save –help`

Files and directories will be saved into the special tar-file `xwin_backup.tar` which is, by default, in the directory `TOPSPINHOME/xwin_backup`.

The *xwinnmr.save* script saves the same files and directories as the nmr_save AU program (see chapter 8.8).

The options for *`xwinnmr.save`* starting from a command prompt are:
`xwinnmr.save` [-options]

   • *`help`*   additional information

- **`path <string>`**   absolute path where backup tar-file `nmr_backup.tar` will be created (backup directory)

- **`restore <string>`**   absolute path where backup tar-file can be found (backup directory); the target directory must also be specified! (see examples below)

- **`replace`**   overwrite existing nmr_backup.tar file

- **`silent`**   do not display any messages

- **`source <string>`**   absolute path to TOPSPIN/XWIN-NMR installation that should be saved

- **`spect <string>`**   spectrometer name (e.g. spect; default is the current name)

For safety reasons the tar-file will not be replaced by executing the ***xwin-nmr.save*** script once again. So if you like to use the script several times, you have to move the xwin_backup.tar file from the directory TOPSPIN-HOME/xwin_backup on a backup medium (floppy, CD ...) and then start the script once again or you have to use the 'replace' option.

21.3 Where Do I Find What?

If you cannot find the required information in this manual, please check the manuals listed below.

Further useful information you can also find in the Release Letter for the respective TOPSPIN version.

- TOPSPIN Users Guide
  Window handling, diplaying data, interactive data manipulation, user interface related items.

- Acquisition Reference
  Description of all acquisition commands, parameters and files.

- Processing Reference
  Description of all processing commands, parameters and files.

- AU Reference
  How to write AU programs. Description of all AU macros, functions and variables. List of Bruker AU programs.

- TOPSPIN PLOT EDITOR
  Printing and plotting of data sets.

- NMR-SIM Experiment Simulator
  Simulation of NMR experiments.

- ICON-NMR Automation Interface
  Comprehensive user interface, tailor made for all your laboratory management
  and control needs.

For further manuals please refer to:

- TOPSPIN → **Help**

- *http://www.bruker-biospin.com/documentation_nmr.html*

- NMR-GUIDE

Chapter 22

Bruker BioSpin addresses

Germany

```
Bruker BioSpin GmbH
Silberstreifen
76287 Rheinstetten
Germany
Tel: +49 (0)721 5161 0
Fax: +49 (0)721 5171 01


Bruker BioSpin
Service & Support Department
Silberstreifen
76287 Rheinstetten
Tel: +49 (0) 721 5161 296
Fax: +49 (0) 721 5161 943
```

http://www.bruker-biospin.com

ftp server: ftp.bruker.de

```
Email: nmr@bruker-biospin.de (sales)
       mbu@bruker.de (service)
       applik@bruker.de (application)
       nmr-software-support@bruker-biospin.de (software)
       license@bruker.de (licenses)
```

USA

```
Bruker BioSpin Corporation
15 Fortune Drive
Manning Road
Billerica, MA. 01821-3991

Tel: +1 978 667 9580 5195 (center)
     +1 978 667 9580 5444 (application)
Fax: +1 978 667 6168 (center)
     +1 978 667 2955 (application)

http://www.bruker-biospin.com
ftp server: ftp.bruker.com

e-mail: applab@bruker.com
        center@bruker.com
        software@bruker.com
```

Switzerland

```
Bruker BioSpin AG
Industriestraße 26
CH-8117 Fällanden

Tel: +41 (44) 8259 111
Fax: +41 (44) 8259 696

web server: www.bruker.ch
e-Mail: epweb@bruker.ch
        all_ap@bruker.ch
```

France

```
Bruker BioSpin S.A.
34, rue de l'industrie
F-67166 Wissembourg/Cedex

Tel: +33 3 88 73 68 00
Fax: +33 3 88 73 68 79

e-Mail: support-rmn@bruker.fr (customer support)
```

England

```
Bruker BioSpin LTD.
Banner lane
Coventry CV4 9GH
Tel: +44 (24) 7685 5200
Fax: +44 (24) 7646 5317

web server: www.bruker.co.uk

e-mail: service@bruker.co.uk
        apps@bruker.co.uk
```

Our webpage

http://www.bruker-biospin.com/contact_us.html

- provides contact adresses of our facilities and offices worldwide